# $[Co(NH_3)_6]^{3+}$

| $O_h$ ($m3m$) | $E$ | $8C_3$ | $6C_2$ | $6C_4$ | $3C_2$ ($=C_4^2$) | $i$ | $6S_4$ | $8S_6$ | $3\sigma_h$ | $6\sigma_d$ | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $A_{1g}$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | | $x^2+y^2+z^2$ |
| $A_{2g}$ | 1 | 1 | −1 | −1 | 1 | 1 | −1 | 1 | 1 | −1 | | |
| $E_g$ | 2 | −1 | 0 | 0 | 2 | 2 | 0 | −1 | 2 | 0 | | $(2z^2-x^2-y^2,$ $\sqrt{3}\ (x^2-y^2))$ |
| $T_{1g}$ | 3 | 0 | −1 | 1 | −1 | 3 | 1 | 0 | −1 | −1 | $(R_x, R_y, R_z)$ | |
| $T_{2g}$ | 3 | 0 | 1 | −1 | −1 | 3 | −1 | 0 | −1 | 1 | | $(xy, xz, yz)$ |
| $A_{1u}$ | 1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 | | |
| $A_{2u}$ | 1 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 | | |
| $E_u$ | 2 | −1 | 0 | 0 | 2 | −2 | 0 | 1 | −2 | 0 | | |
| $T_{1u}$ | 3 | 0 | −1 | 1 | −1 | −3 | −1 | 0 | 1 | 1 | $(x, y, z)$ | |
| $T_{2u}$ | 3 | 0 | 1 | −1 | −1 | −3 | 1 | 0 | 1 | −1 | | |

# Molecole ipervalenti: $SF_6$ (gruppo $O_h$)

| $O_h$ | $E$ | $8C_3$ | $6C_2$ | $6C_4$ | $3C_2$ $(= C_4^2)$ | $i$ | $6S_4$ | $8S_6$ | $3\sigma_h$ | $6\sigma_d$ |
|---|---|---|---|---|---|---|---|---|---|---|
| $A_{1g}$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_{2g}$ | 1 | 1 | −1 | −1 | 1 | 1 | −1 | 1 | 1 | −1 |
| $E_g$ | 2 | −1 | 0 | 0 | 2 | 2 | 0 | −1 | 2 | 0 |
| $T_{1g}$ | 3 | 0 | −1 | 1 | −1 | 3 | 1 | 0 | −1 | −1 |
| $T_{2g}$ | 3 | 0 | 1 | −1 | −1 | 3 | −1 | 0 | −1 | 1 |
| $A_{1u}$ | 1 | 1 | 1 | 1 | 1 | −1 | −1 | −1 | −1 | −1 |
| $A_{2u}$ | 1 | 1 | −1 | −1 | 1 | −1 | 1 | −1 | −1 | 1 |
| $E_u$ | 2 | −1 | 0 | 0 | 2 | −2 | 0 | 1 | −2 | 0 |
| $T_{1u}$ | 3 | 0 | −1 | 1 | −1 | −3 | −1 | 0 | 1 | 1 |
| $T_{2u}$ | 3 | 0 | 1 | −1 | −1 | −3 | 1 | 0 | 1 | −1 |

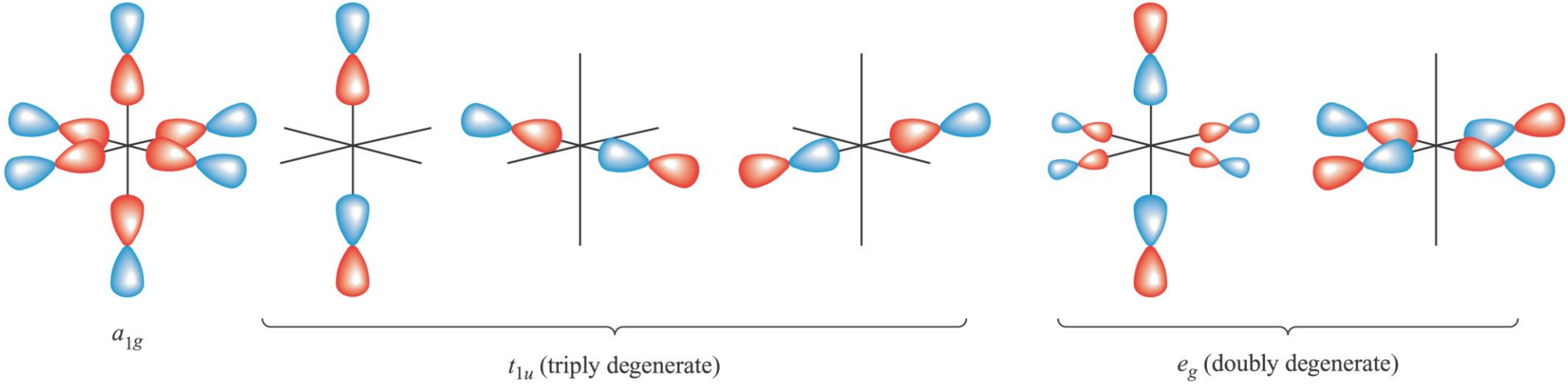
| $E$ | $8C_3$ | $6C_2$ | $6C_4$ | $3C_2$ | i | $6S_4$ | $8S_6$ | $3\sigma_h$ | $6\sigma_d$ |
|---|---|---|---|---|---|---|---|---|---|
| 6 | 0 | 0 | 2 | 2 | 0 | 0 | 0 | 4 | 2 |

sei $2p_z$ radiali =

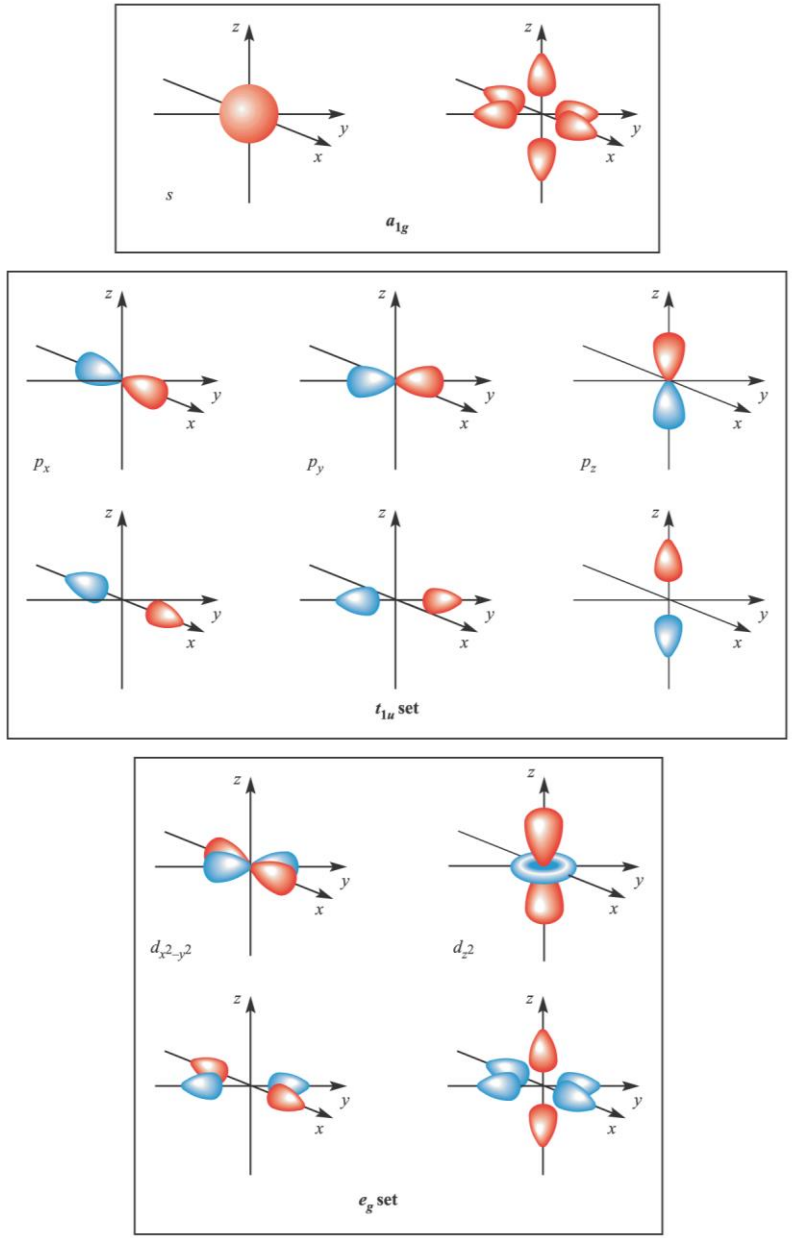
sei *lone pairs* delle molecole di $NH_3$

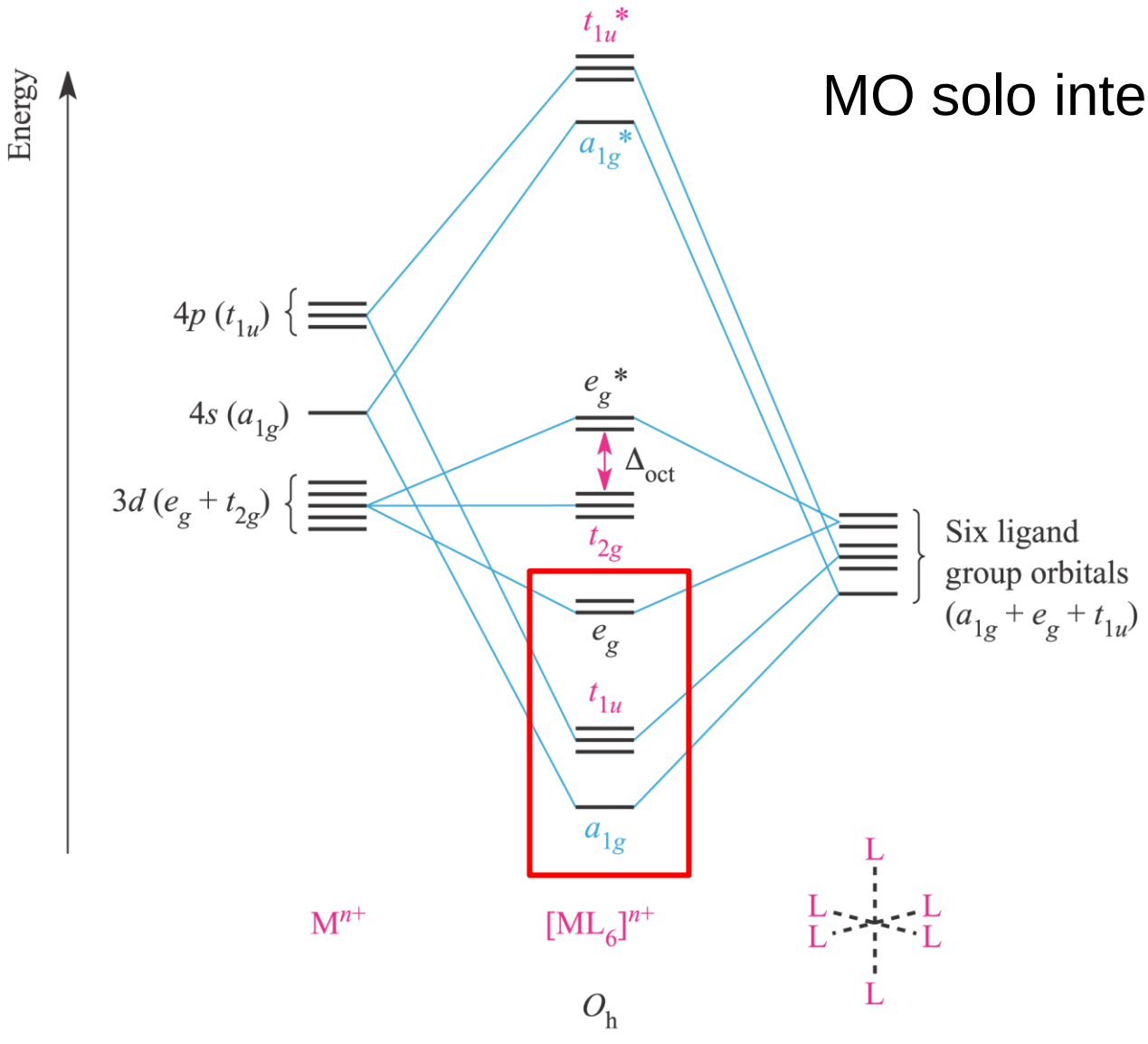
$$A_{1g} + T_{1u} + E_g$$

# LGO del gruppo $F_6$ in $SF_6$



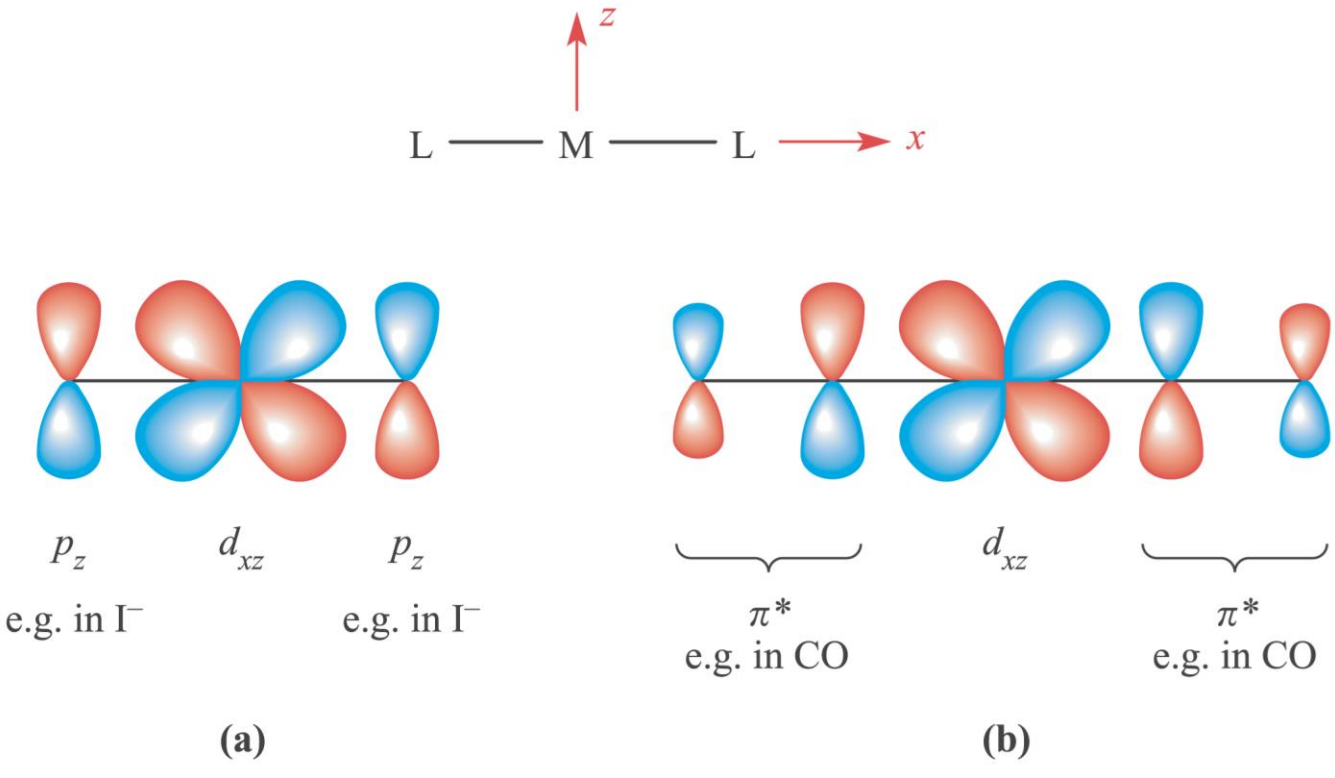
# LGO di $[Co(NH_3)_6]^{3+}$






La sovrapposizione tra gli LGO e gli orbitali s e p del metallo è maggiore di quella con gli orbitali d, e quindi gli MO $a_{1g}$ e $t_{1u}$ saranno stabilizzati più degli $e_g$.

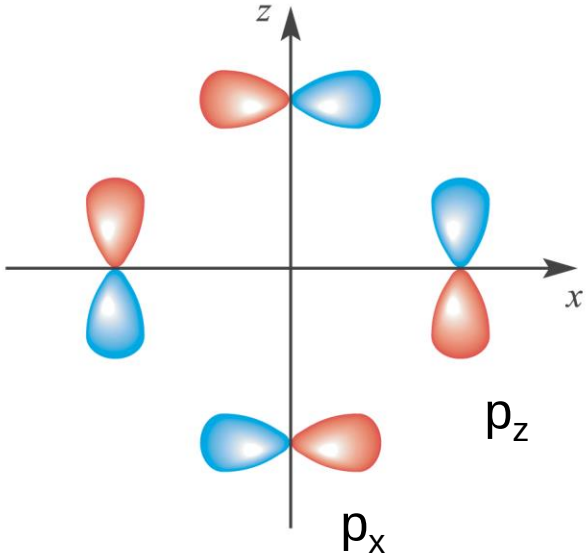
# Interazioni π




π-donatore

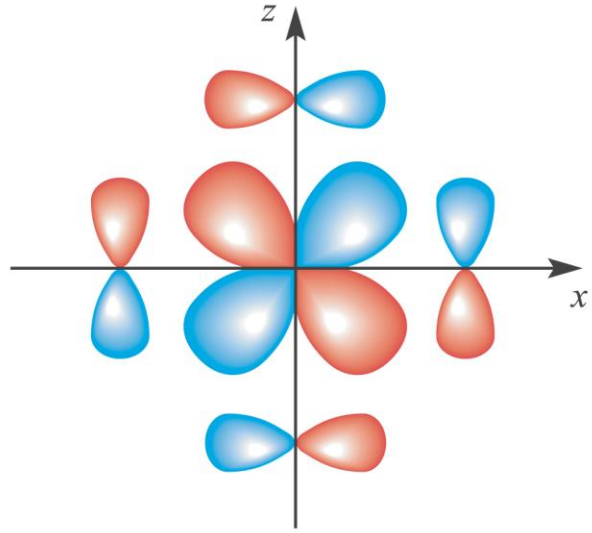
π-accettore
(retrodonazione π)

# LGO π in un piano di un ottaedro

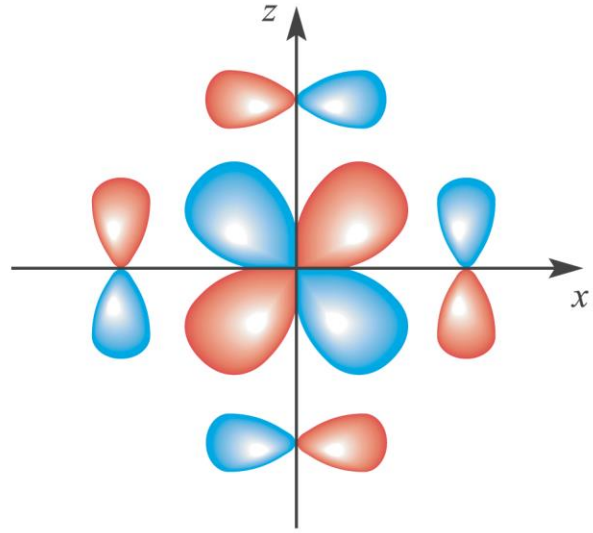



$p_z$

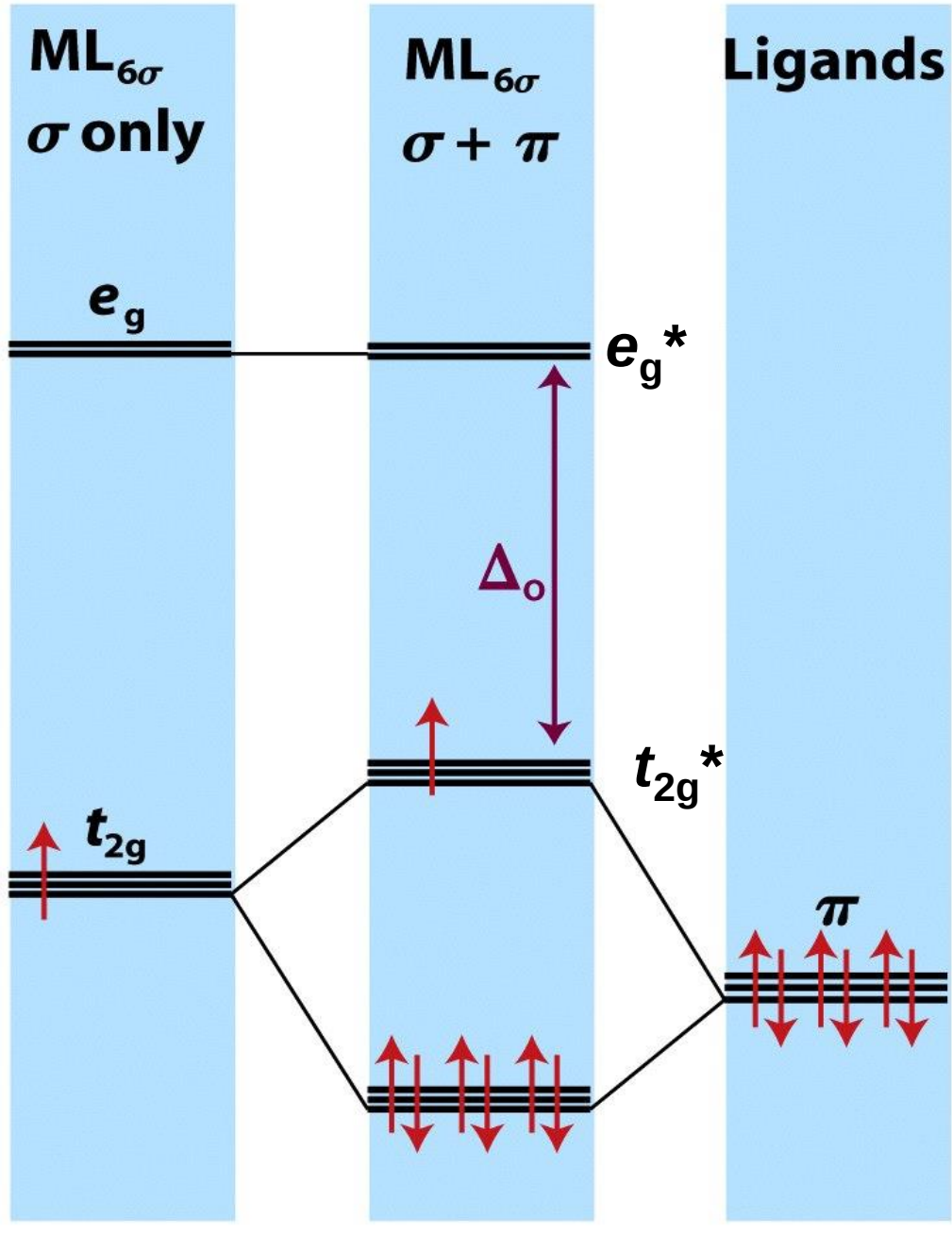
$p_x$




combinazione legante

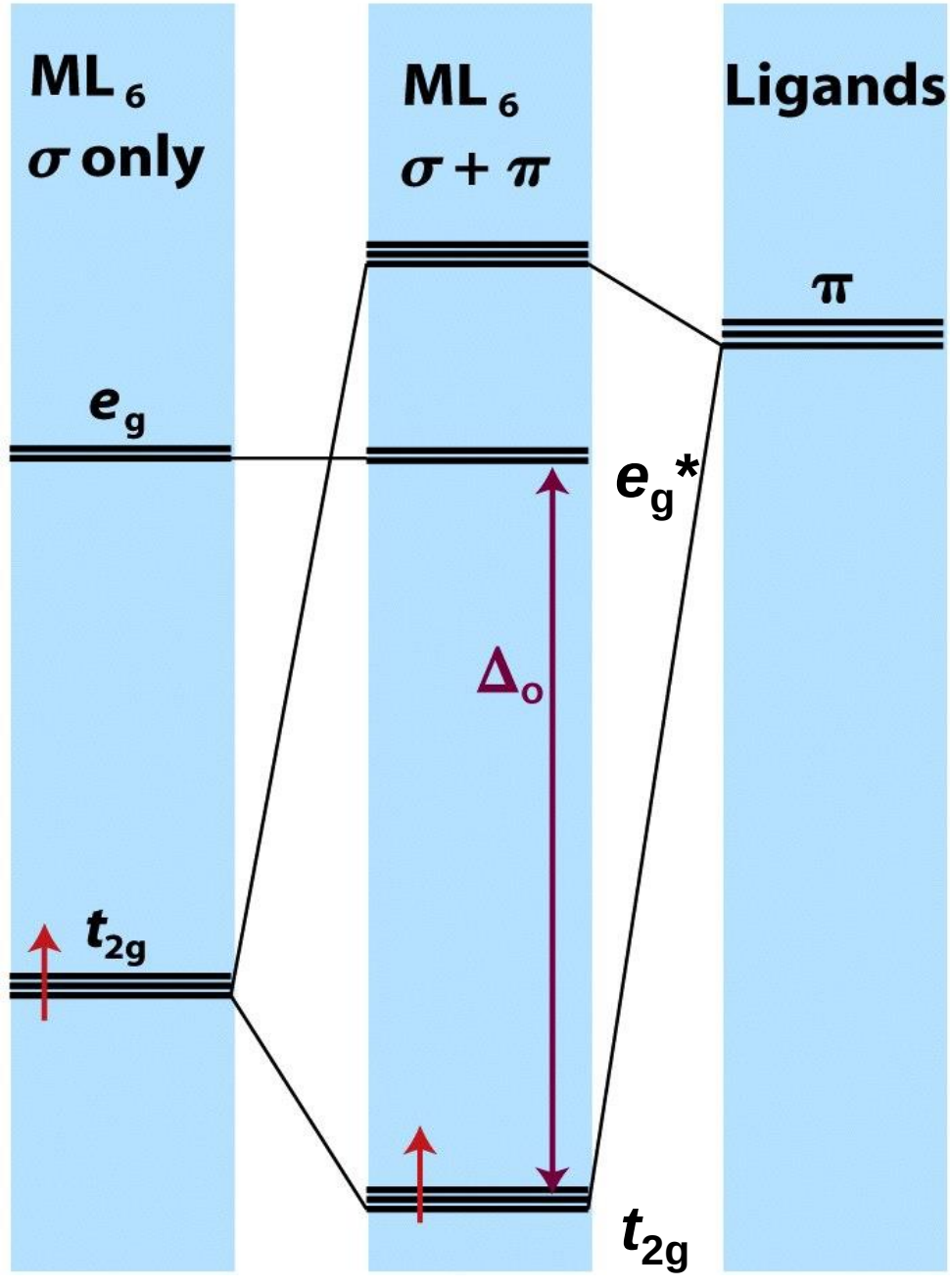



combinazione antilegante



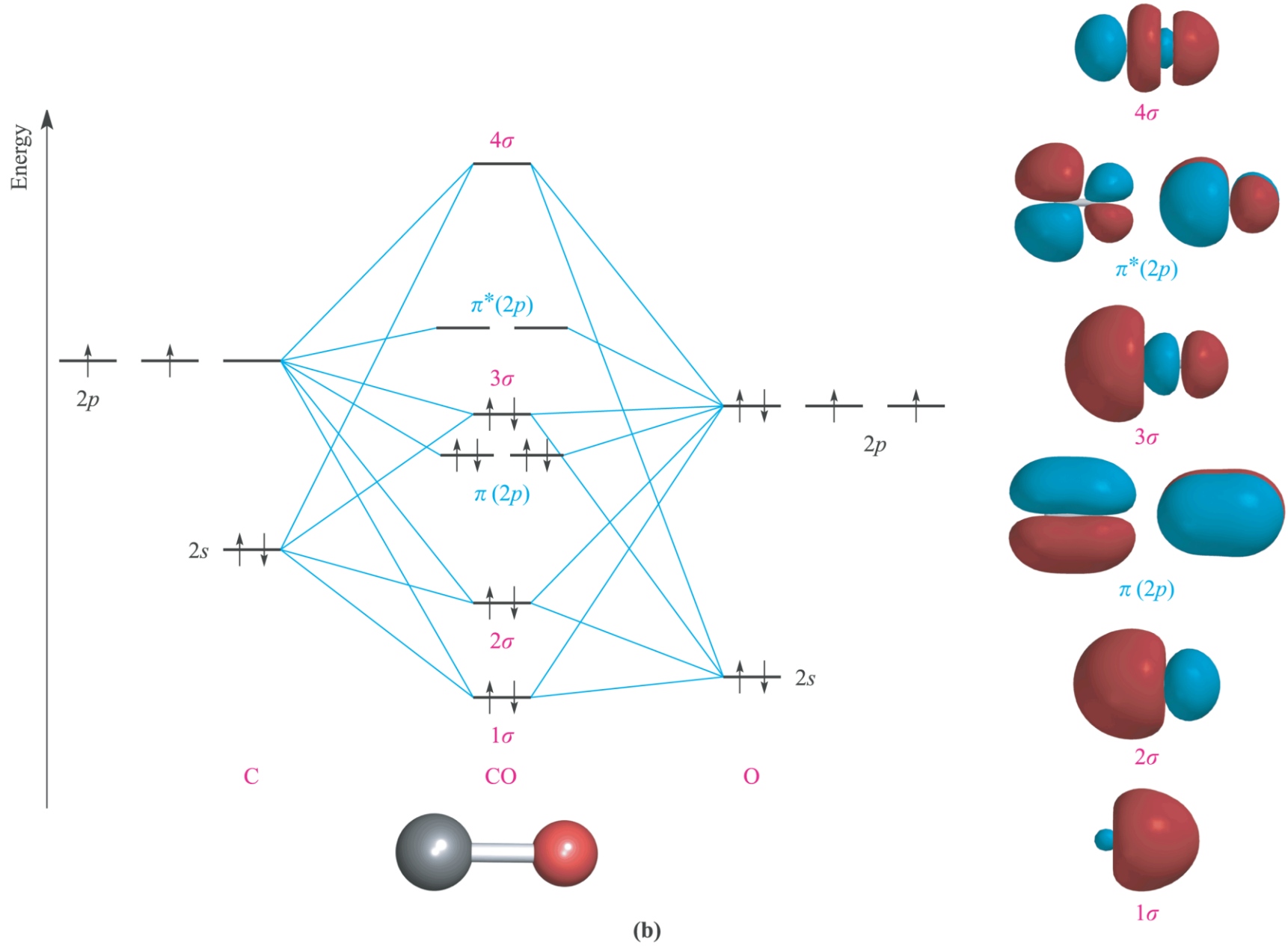

π-donatore
e.g. $[CoF_6]^{3-}$

LGO $t_{2g}$
($t_{1u}$ $t_{2u}$ $t_{1g}$)

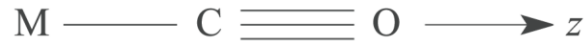


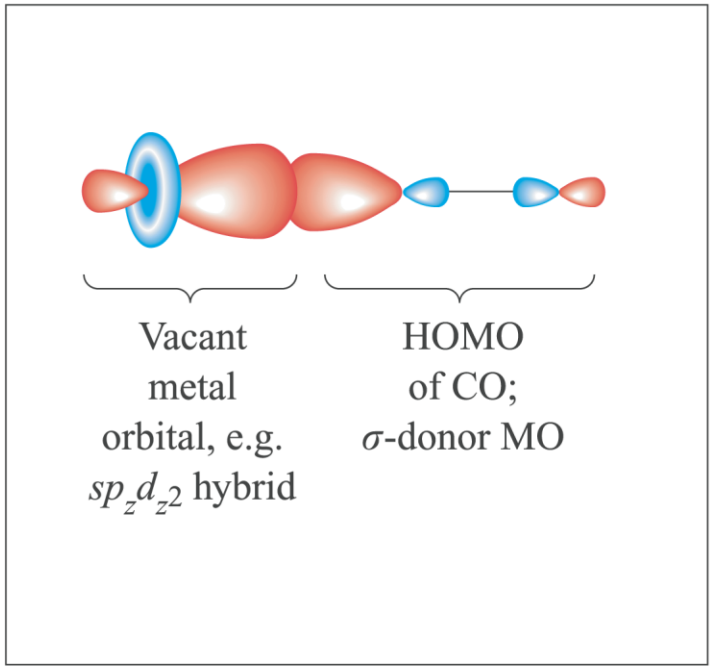

π-accettore

*Leganti π-accettori stabilizzano metalli in basso stato di ossidazione*

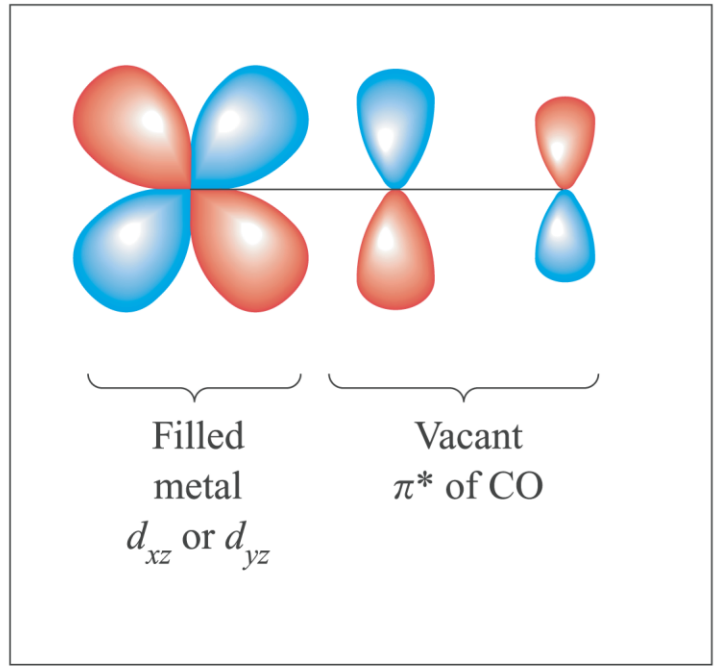



(b)




CO-to-M donation
(a)




M-to-CO back-donation
(b)

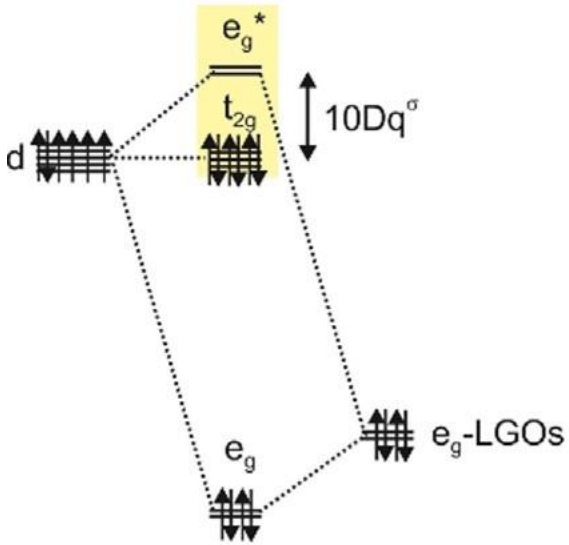
# Serie spettrochimica dei leganti

$I^- < Br^- < S^{2-} < NCS^- < Cl^- < F^- < OH^- < ox^{2-} \approx H_2O <$
$NCS^- < NH_3 < en < bpy < phen < CH_3^- < CN^- < CO$

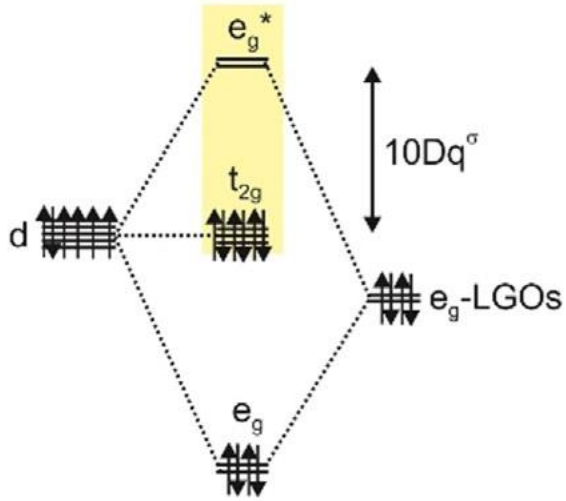
**Campo debole** **Campo forte**

$\pi$ donatori < $\pi$ donatori deboli < nessun contributo $\pi$ < $\pi$ accettori

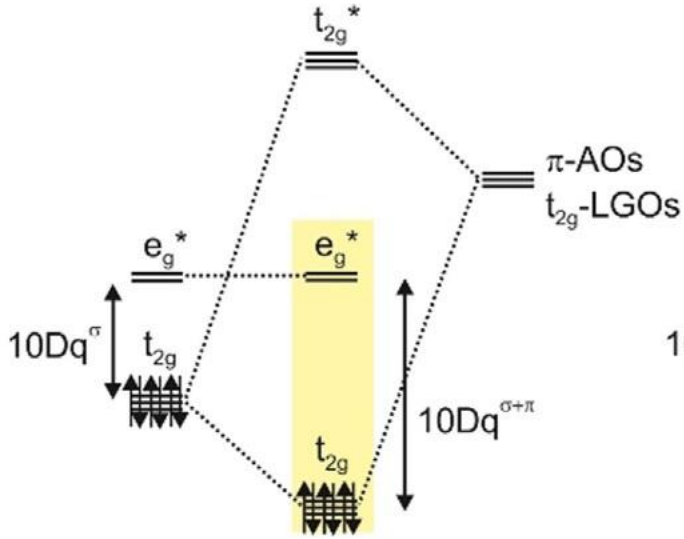
(a) weak σ-donor ligands



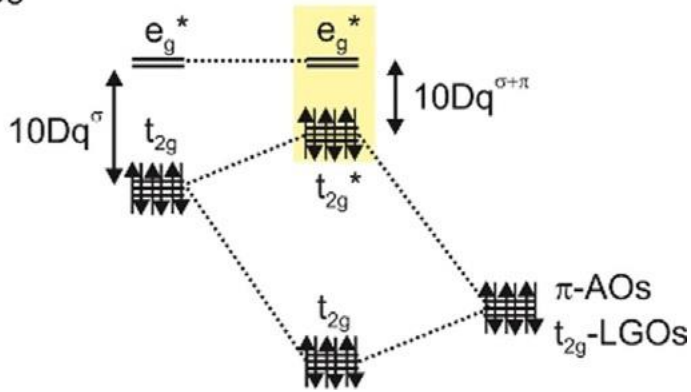

(b) strong σ-donor ligands




(c) π-acceptor ligands




(d) π-donor ligands



# Effetto del contributo π nei planari quadrati