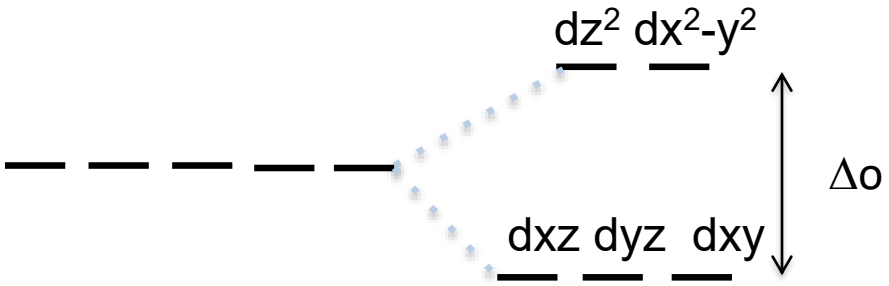
Spectrochemical Series: how to predict relative differences in Δo and what complexes are LS vs HS



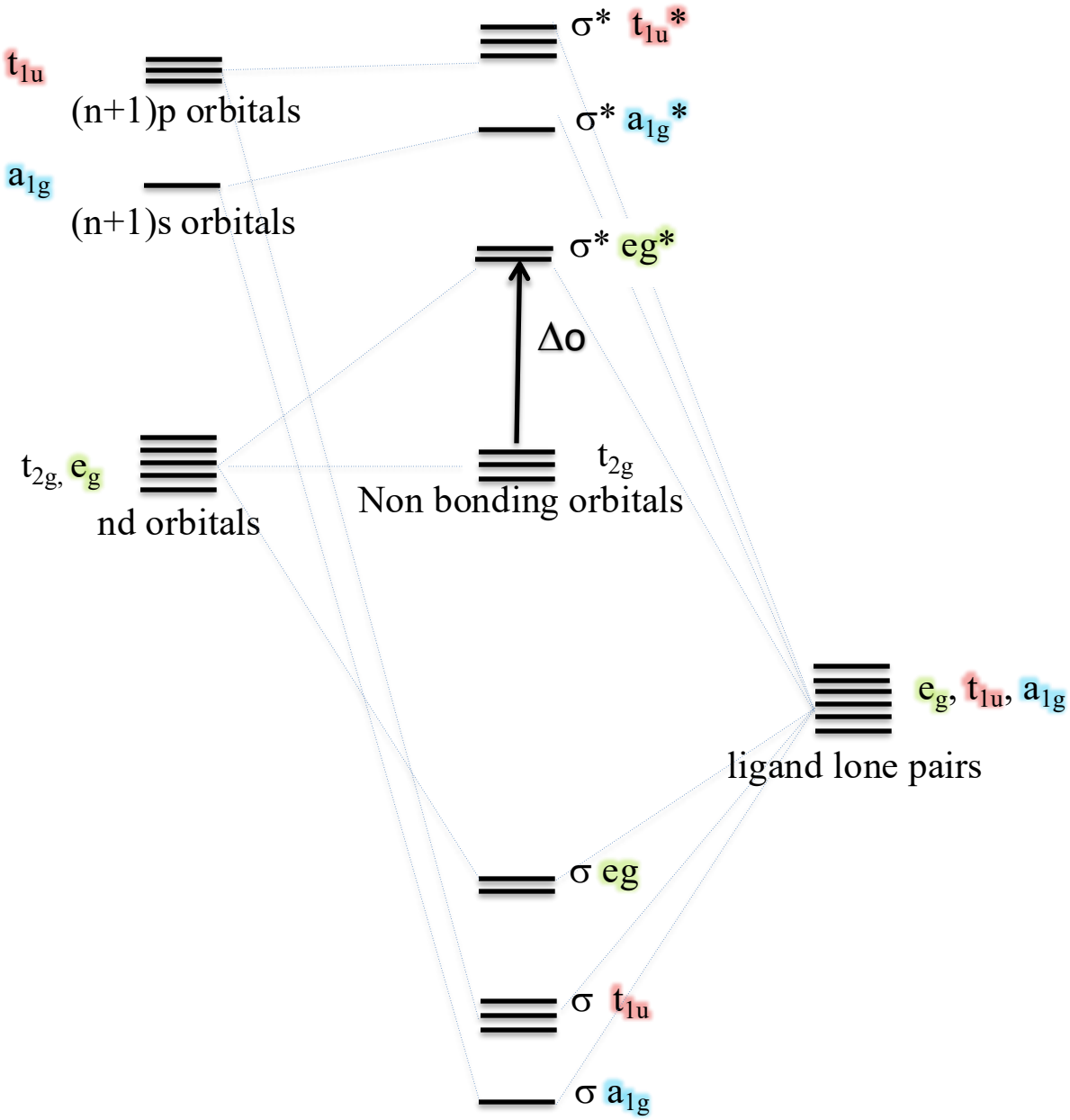
For a common ligand: $Mn^{2+} < Ni^{2+} < Co^{2+} < Fe^{2+} < V^{2+} < Fe^{3+} < Cr^{3+} < V^{3+} < Co^{3+} < Mn^{4+} < Mo^{3+} < Rh^{3+} < Ru^{3+} < Pd^{4+} < Pt^{4+}$ Strong field, Larger Δo leads to low spin complex!

For a common metal: $I^- < Br^- < \underline{S}CN^- < Cl^- < NO_3^- < N_3^- < F^- < OH^- < H_2O < SCN^- <$ py < NH_3 < en < bipy < phen < NO_2^- < PPh3 < CN^- < CO Strong field, Larger Δo, leads to low spin complex!

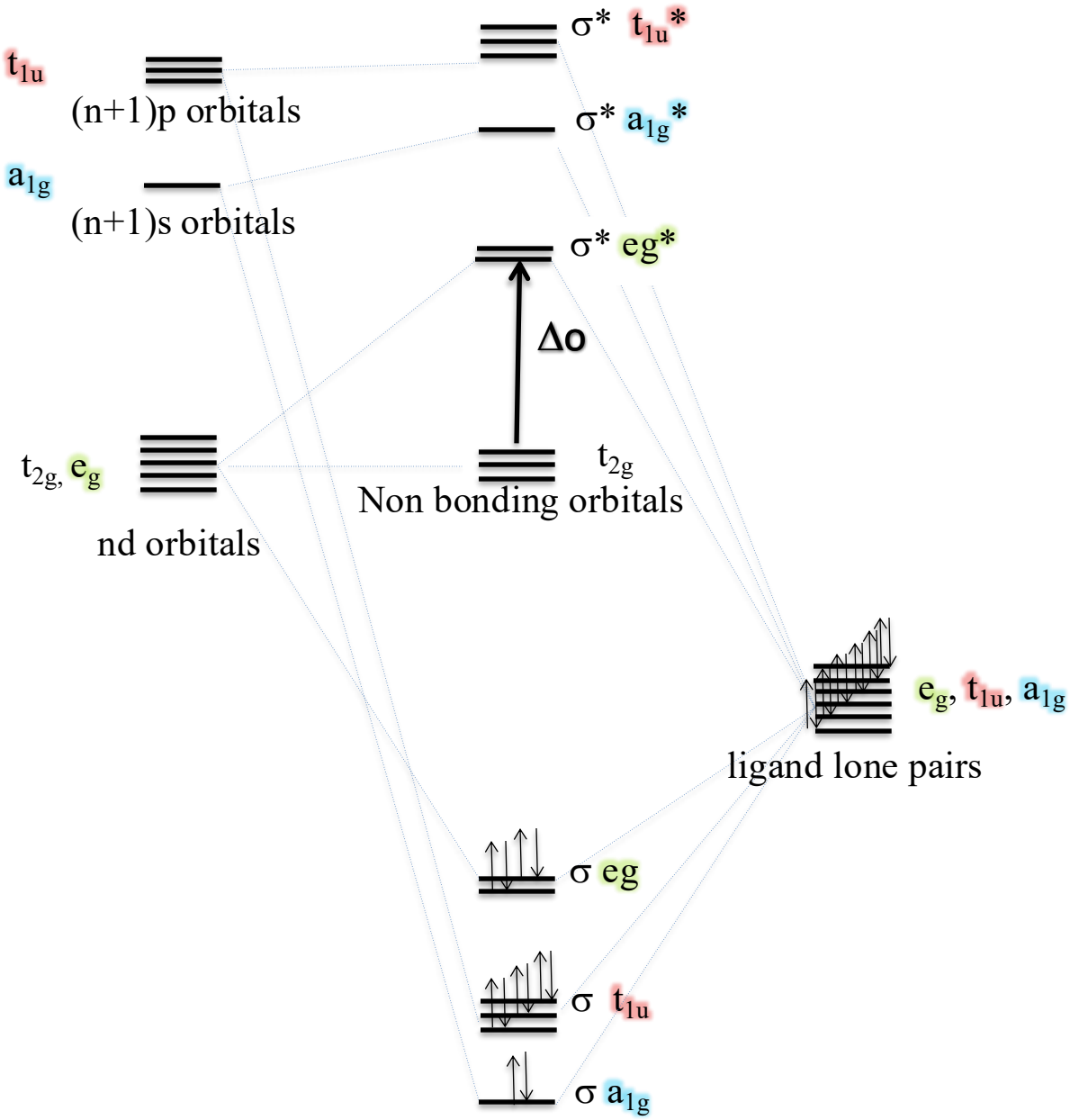
Table: Δo for various metals and ligands in units of 1000 cm^{-1}

	Ions	Ligands				
		Cl^-	H_2O	NH_3	en	CN^-
d^3	Cr^{3+}	13.7	17.4	21.5	21.9	26.6
d^5	Mn^{2+}	7.5	8.5		10.1	30
	Fe^{3+}	11.0	14.3			(35)
d^6	Fe^{2+}		10.4			(32.8)
	Co^{3+}		(20.7)	(22.9)	(23.2)	(34.8)
	Rh^{3+}	(20.4)	(27.0)	(34.0)	(34.6)	(45.5)
d^8	Ni^{2+}	7.5	8.5	10.8	11.5	

σ bonding in metal coordination complexes ML_6

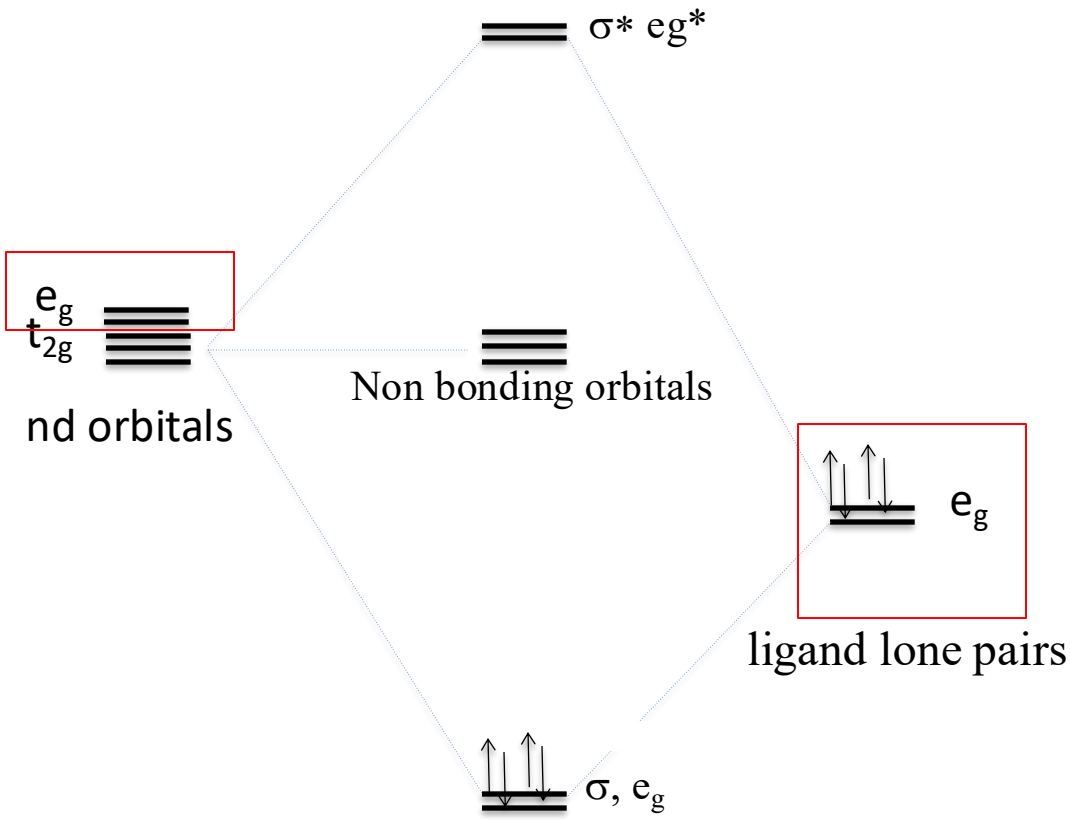


σ bonding in metal coordination complexes ML_6 and filling the molecular orbitals



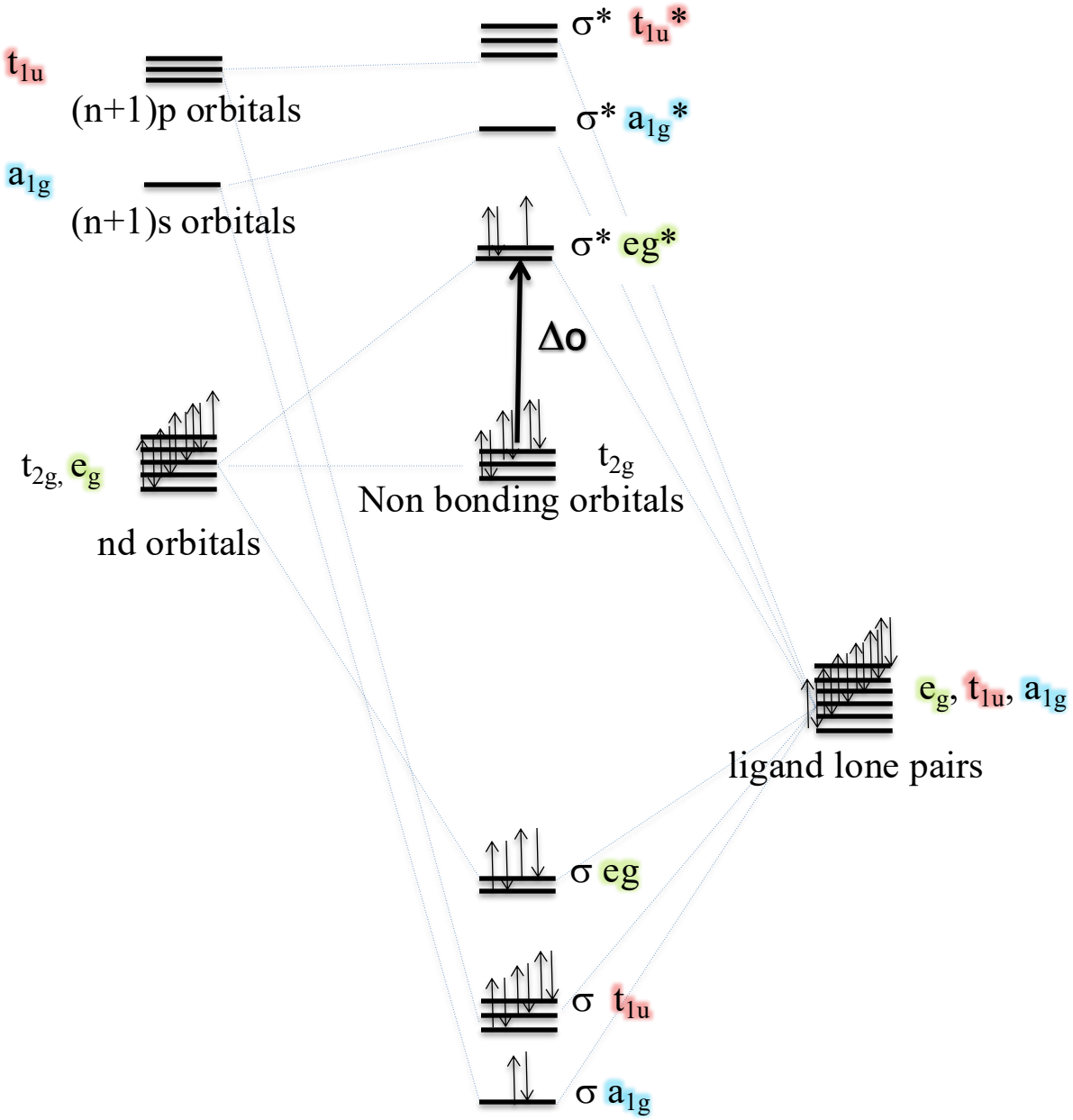
σ bonding in metal coordination complexes ML_6

Simplified MO diagram $[ML_6]^{n+}$

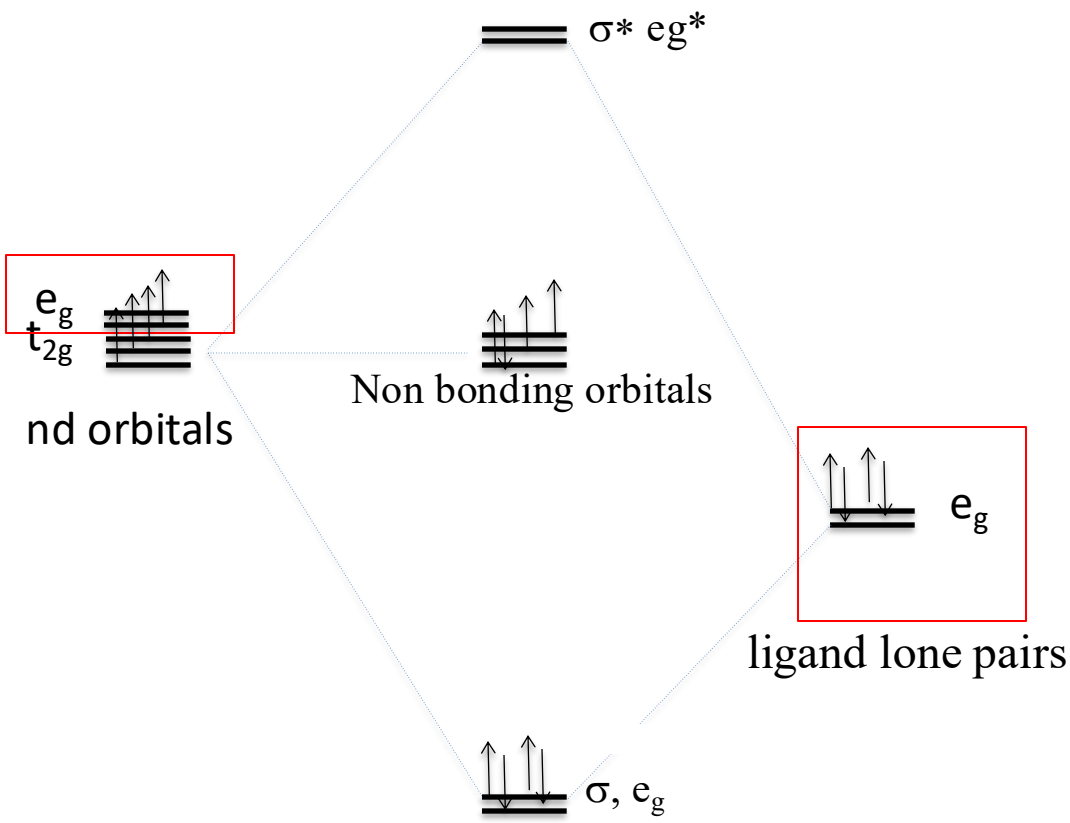


σ bonding in metal coordination in an octahedral complexes containing Cu^{2+}

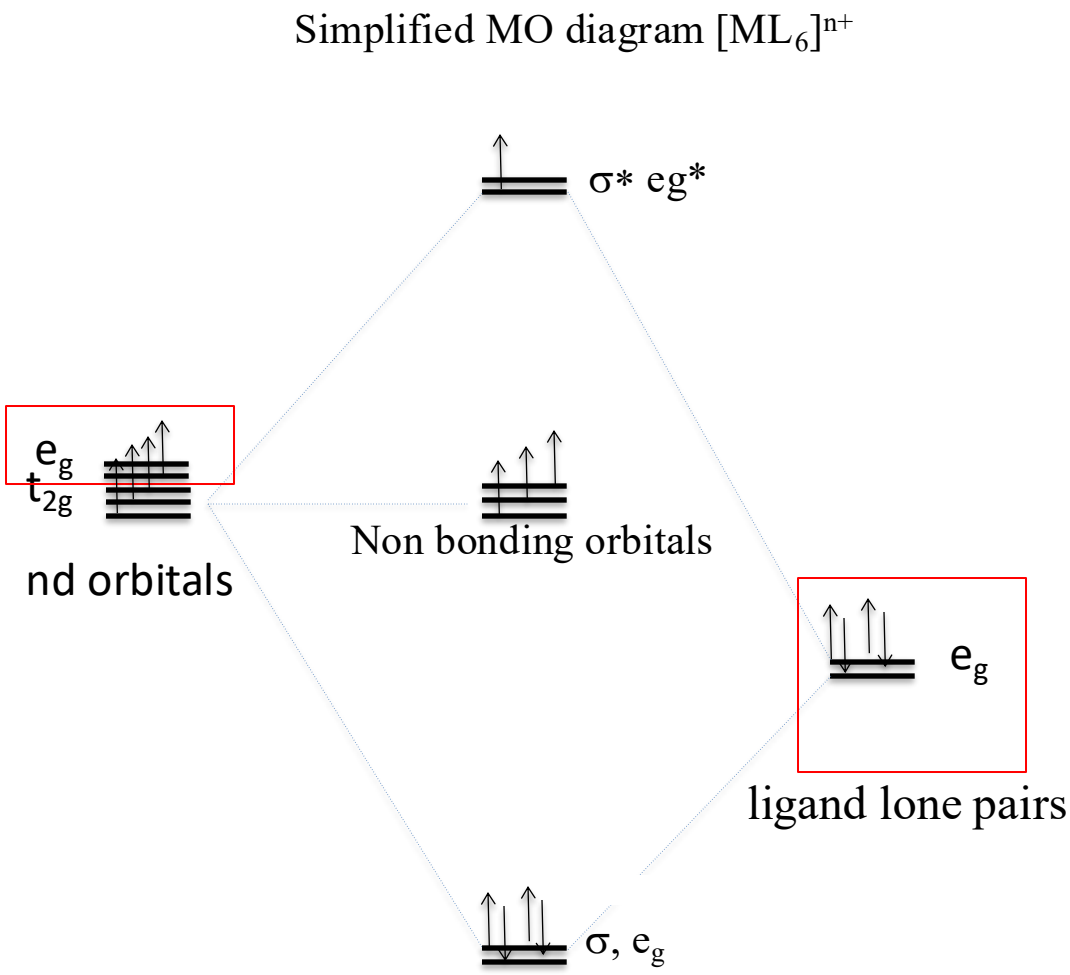
Assuming octahedral geometry



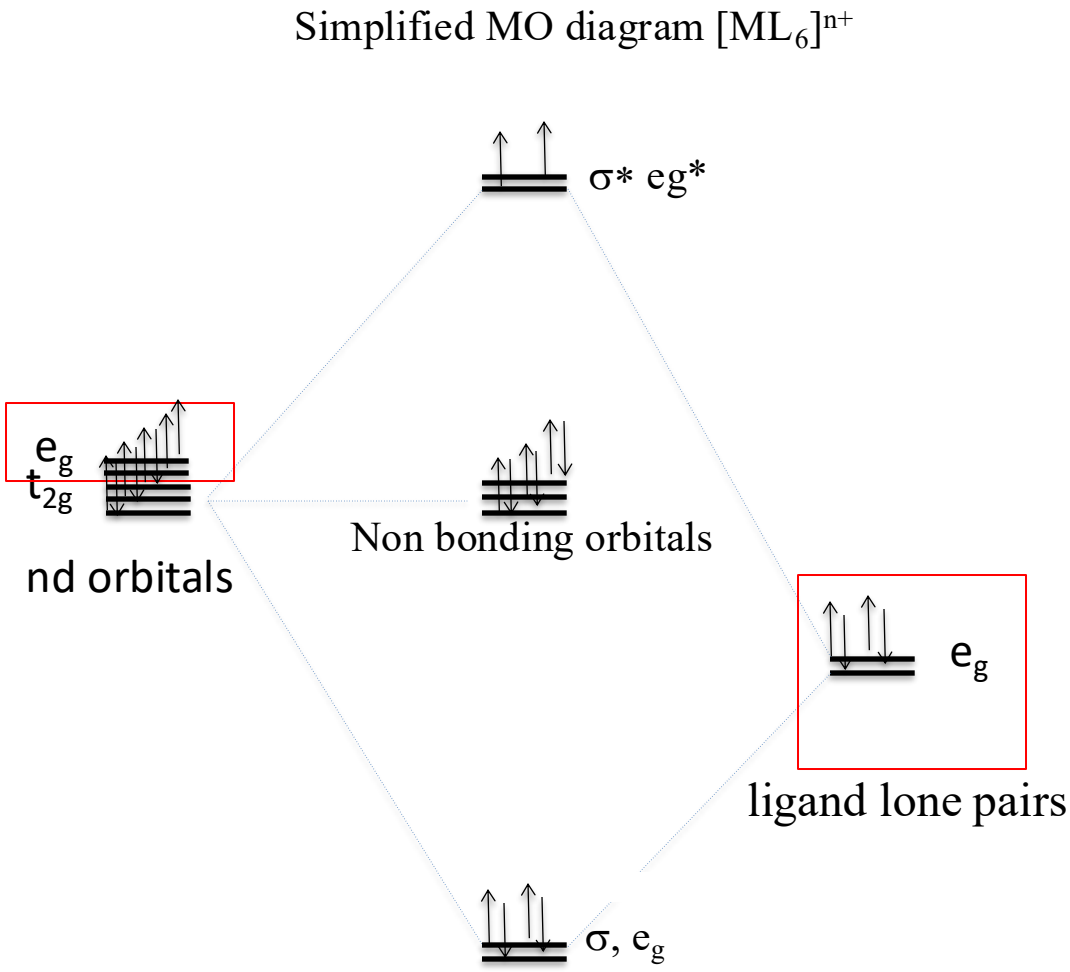
σ bonding in metal coordination complexes ML_6, d^4 complex



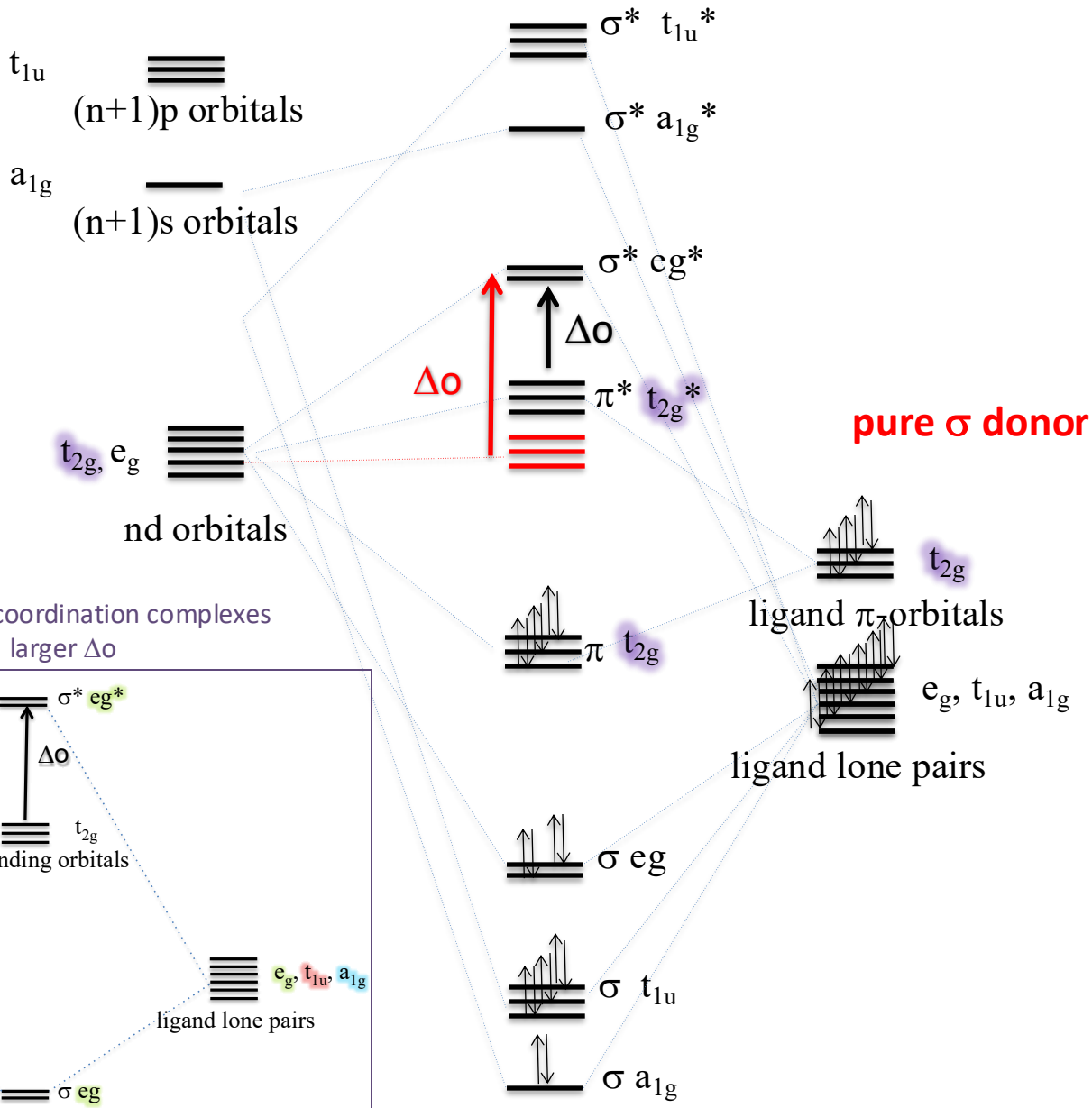
σ bonding in metal coordination complexes ML_6, d^4 complex



σ bonding in metal coordination complexes ML_6, d^8 complex

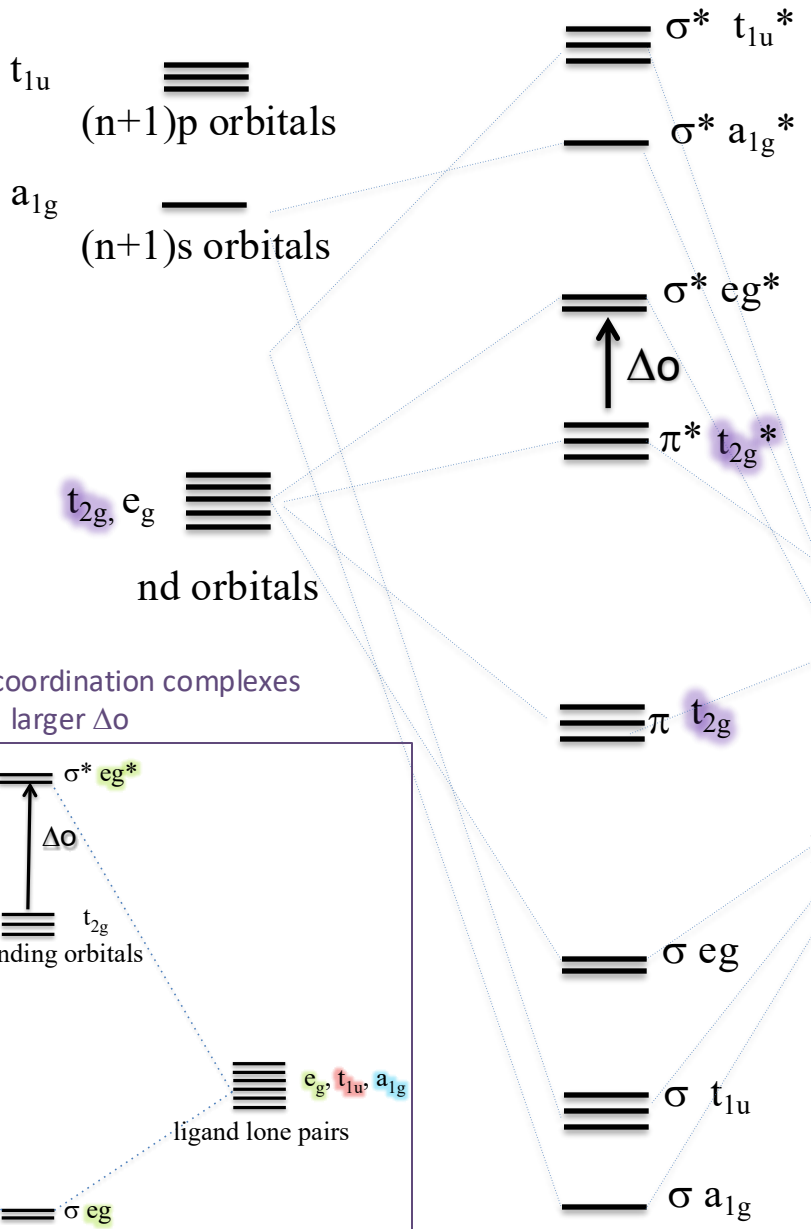


π-donation in ML_6 coordination complexes



σ-donation in ML_6 coordination complexes have a larger Δo

π-donation in ML_6 coordination complexes



Common π-donating ligands include:

I^-, Br^-,Cl^-, F^-, and H_2O

These are commonly found on the far left of the spectrochemical series and give rise to a weak field and hence high-spin complexes.

$I^- < Br^- < SCN^- < Cl^- < NO_3^- < N_3^- < F^- < OH^- < H_2O < SCN^- < py < NH_3 < en < bipy < phen < NO_2^- < PPh_3 < CN^- < CO$

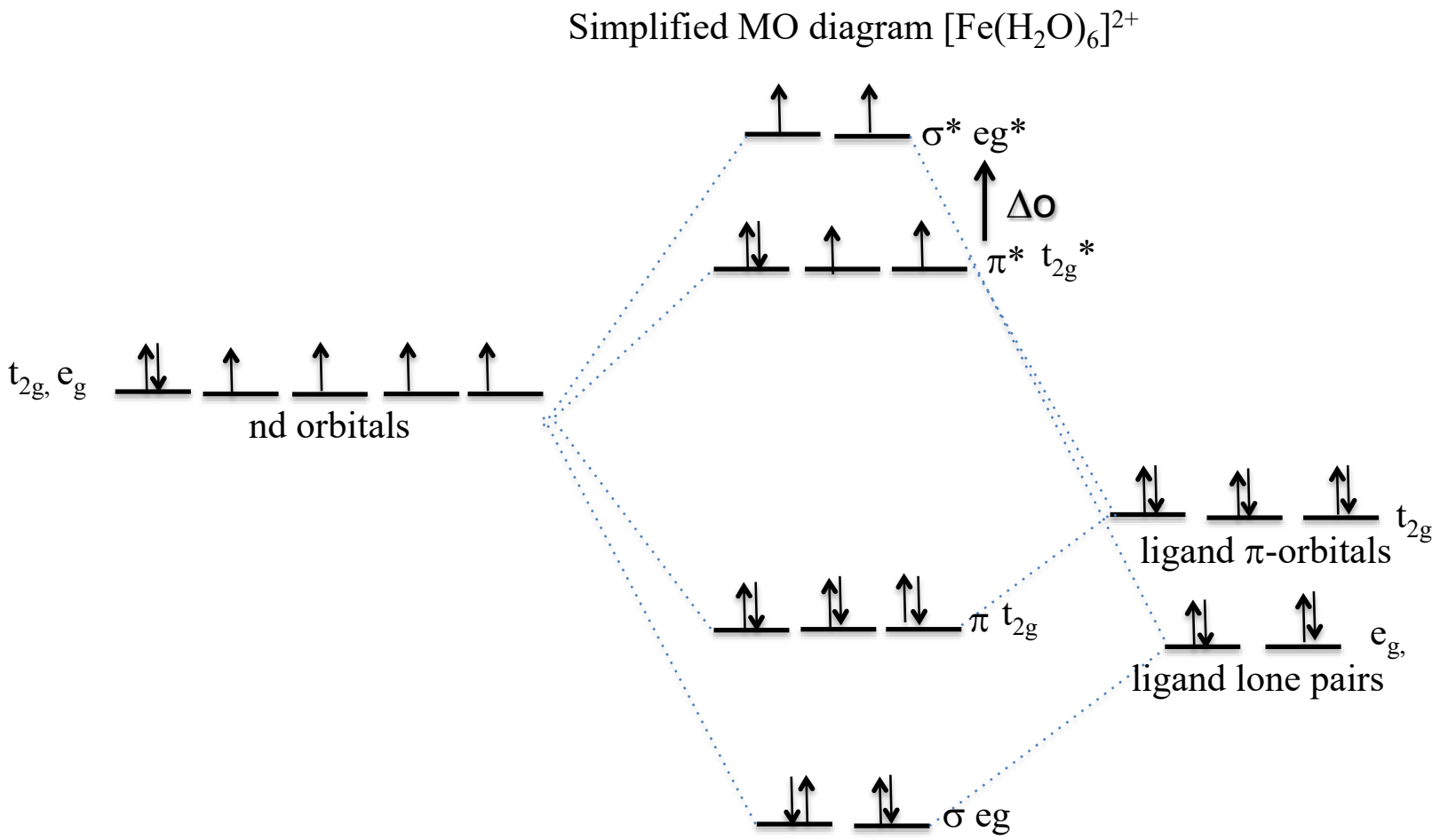
Smaller Δo leads to high spin complex!

L7-L9

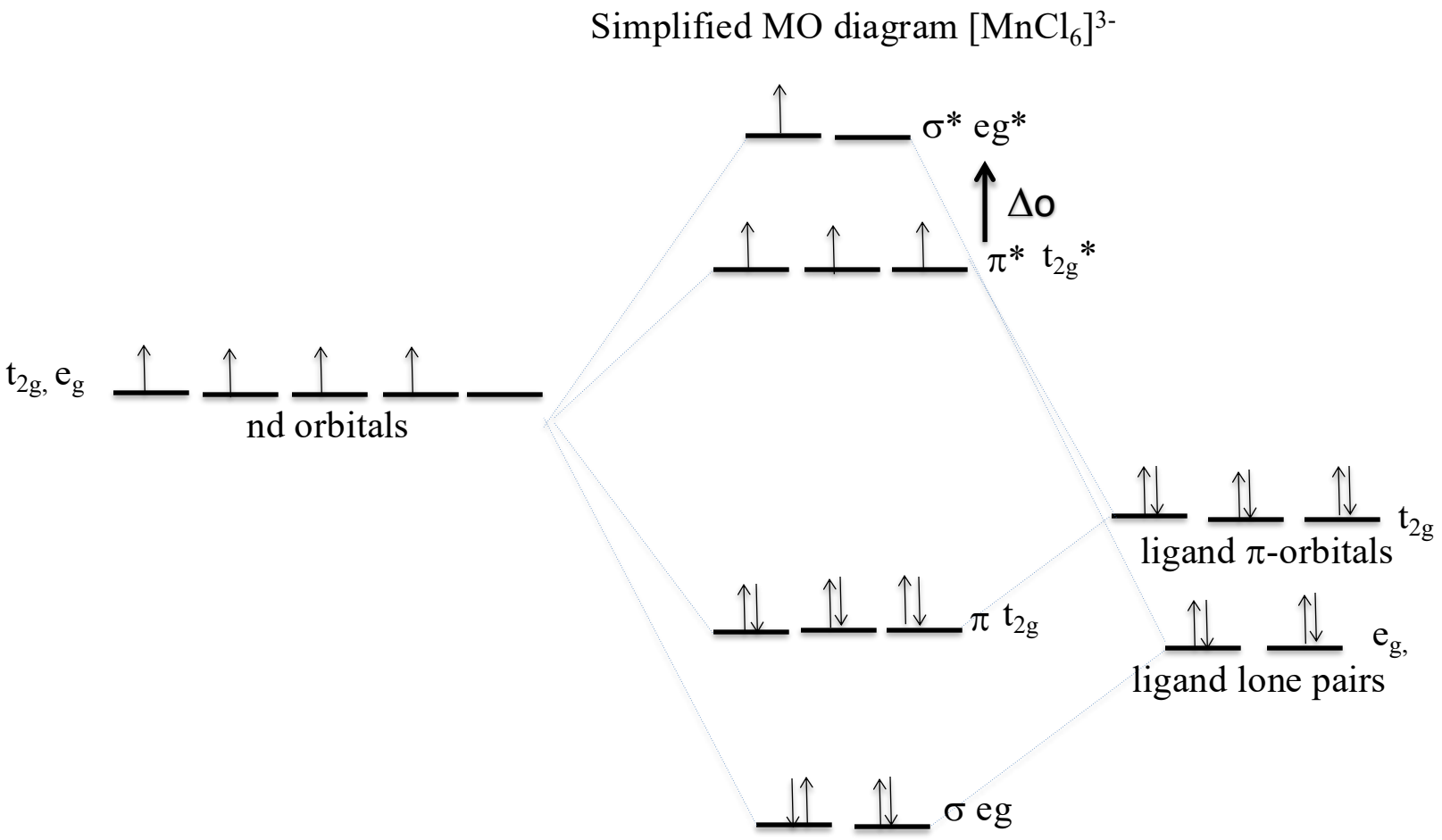
L1-L6

σ-donation in ML_6 coordination complexes have a larger Δo

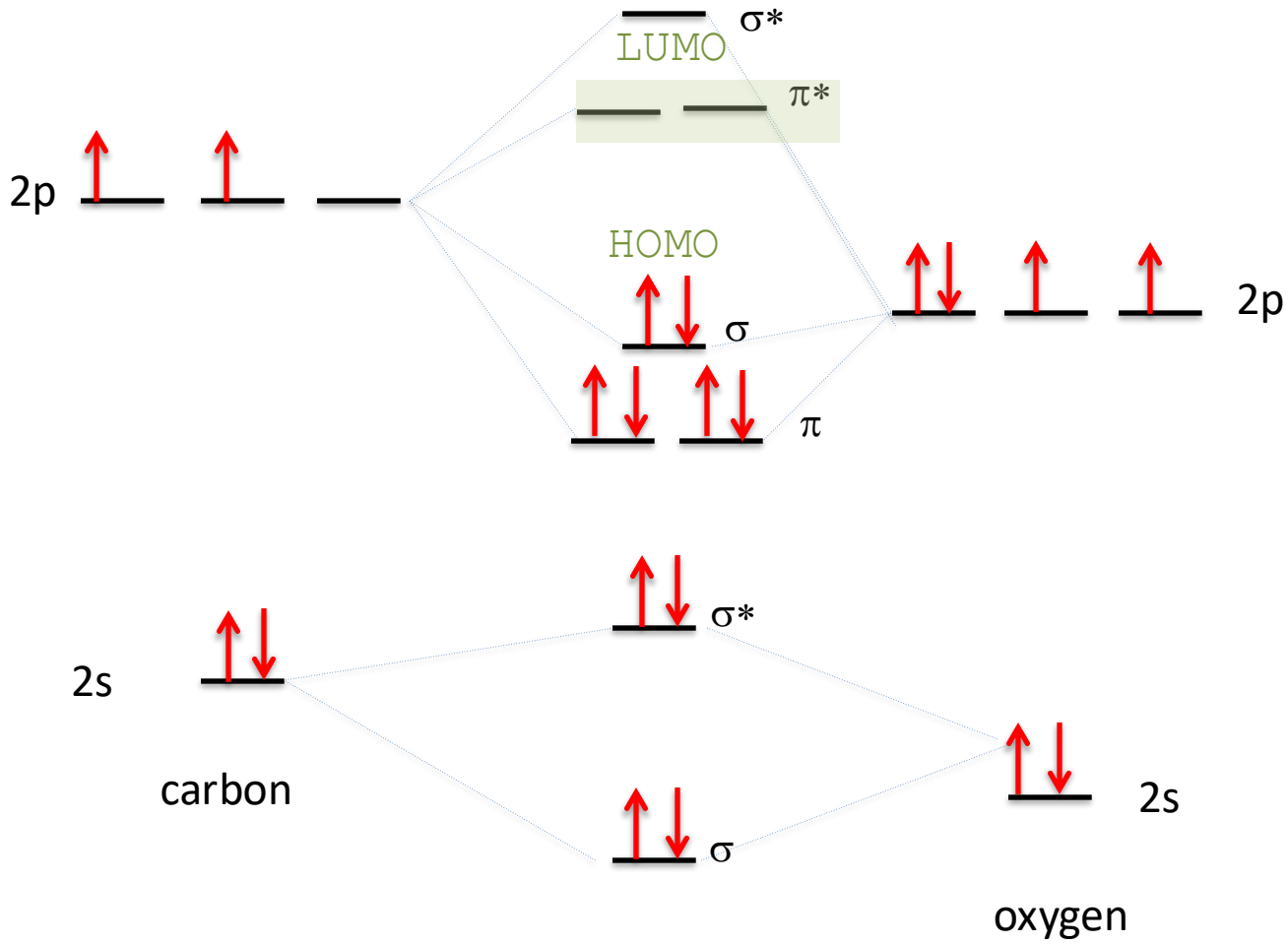
π-donation in ML_6 coordination complexes



π-donation in ML_6 coordination complexes



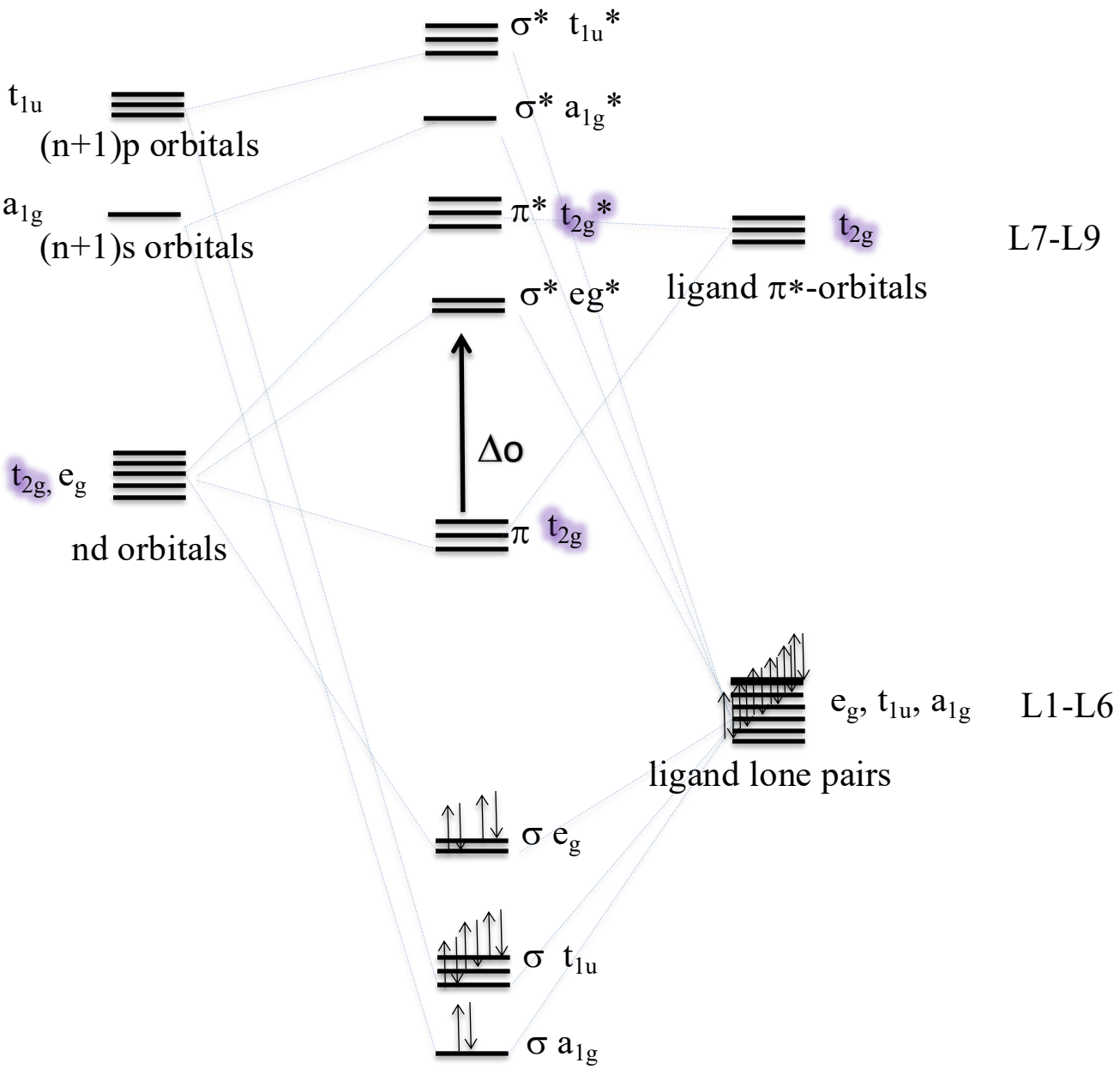
Molecular Orbital Diagram for CO



Bond Order is = 3.0.

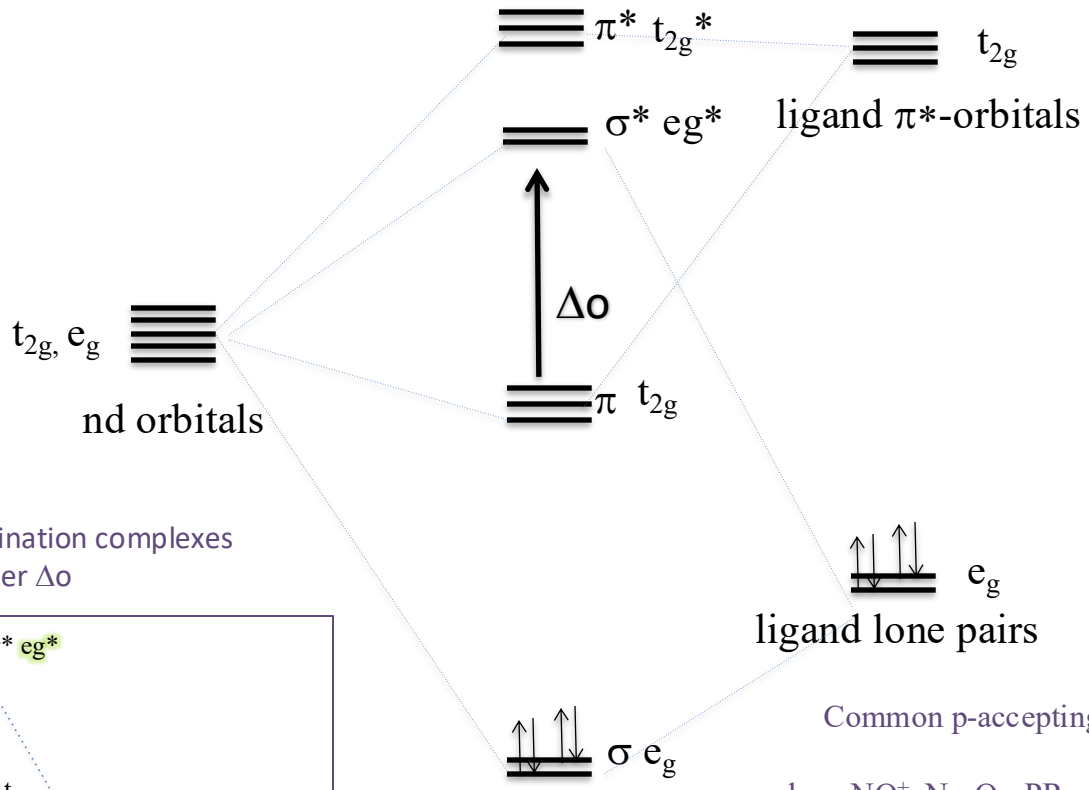
B. O. = ((# bonding e-) –(# nonbonding e-))/ 2

π-acceptor in ML_6 coordination complexes

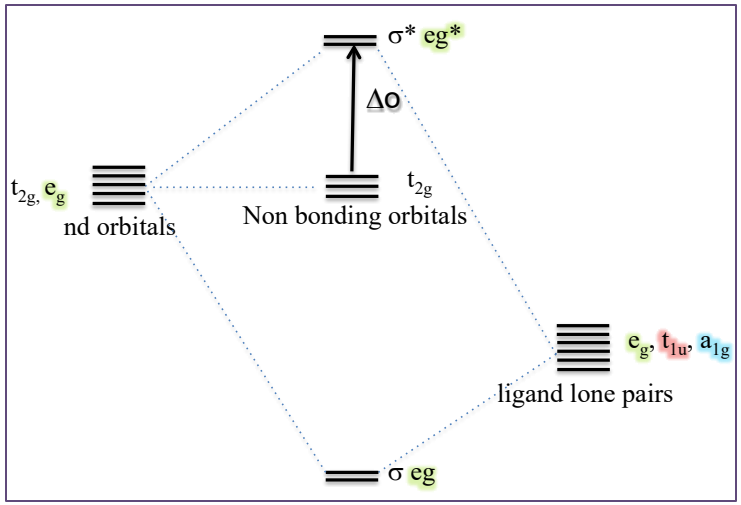


π-acceptor in ML_6 coordination complexes

Simplified MO diagram for π-acceptor



σ-donation in ML_6 coordination complexes have a smaller Δo



Common p-accepting ligands include:

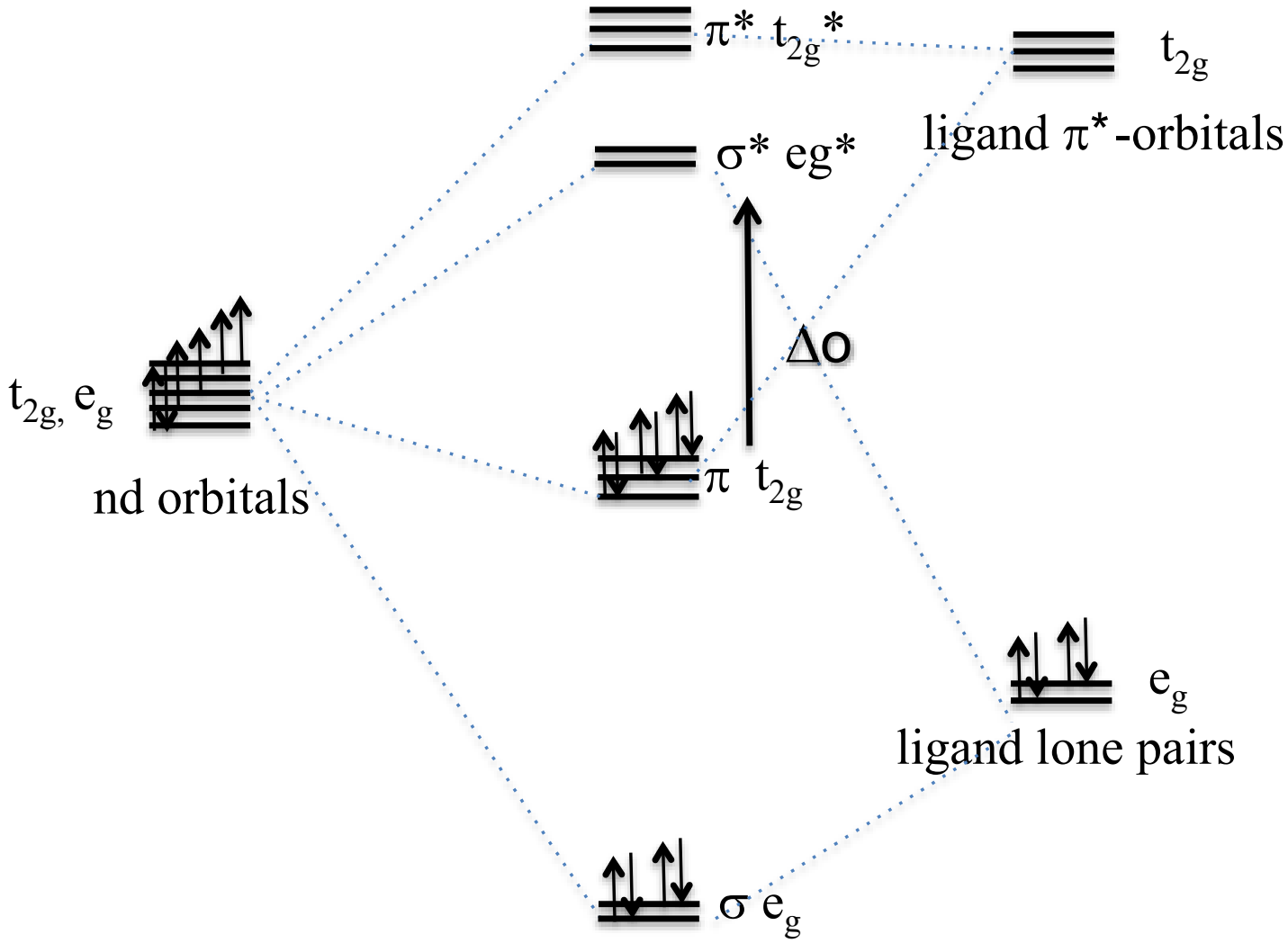
phen, NO^+, N_2, O_2, PR_3, CO, CN- and alkenes

These are commonly found on the far right of the spectrochemical series and give rise to a strong field and hence low-spin complexes.

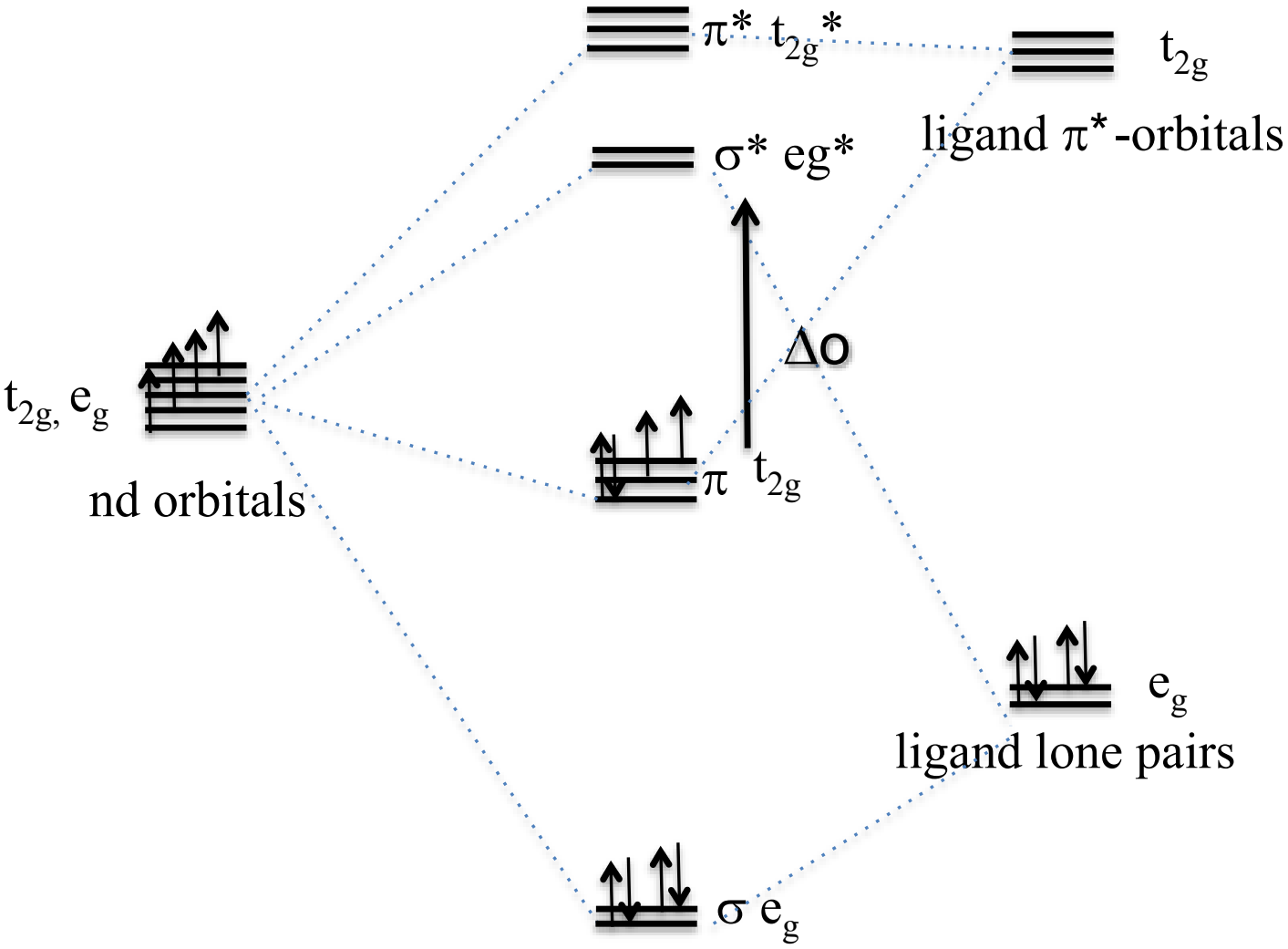
$I^- < Br^- <$ SCN- $< Cl^- < NO_3^- < N_3^- < F^- < OH^- < H_2O <$ SCN- $<$ py $< NH_3 <$ en $<$ bipy $<$ phen $< NO_2^- < PPh_3 < CN^- <$ CO

Larger Δo leads to low-spin complex!

Co^{3+} with a π-acceptor ligand



Cr^{2+} with a π-acceptor ligand



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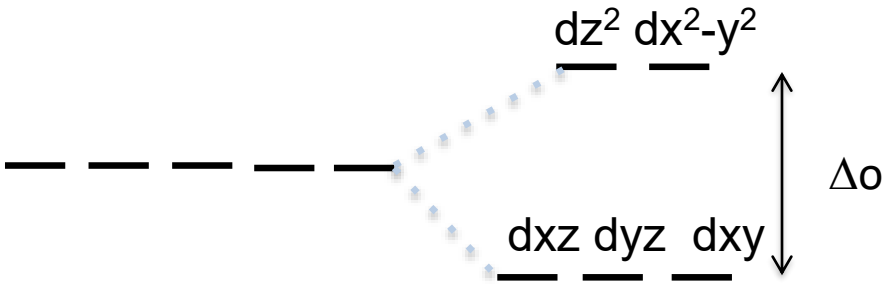

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