(28) **Today**

Section 10.1 Experimental Data Used in when Describing Bonding in Coordination Compound

Section 10.2 Crystal Field Theory

Next Class (29)

Section 10.2 Crystal Field Theory

Section 10.3 Ligand Field Theory

(30) **Second Class from Today**

Section 10.3 Ligand Field Theory

Third Class from Today (31)

Section 10.5 The Jan-Teller Effect

Chap 12

S is the total of the magnetic spin quantum numbers
L is the total of the orbital angular momentum quantum numbers

for N $1s^2\ 2s^2\ 2p^3$

$S = \frac{1}{2} + \frac{1}{2} + \frac{1}{2} = \frac{3}{2}$

$m_l = 1 \quad m_l = 0 \quad m_l = -1$

$L = 1 + 0 + -1 = 0$

$2p^3$ ↑ ↑ ↑

$2s^2$ ↑↓ $m_l = 0$

$1s^2$ ↑↓ $m_l = 0$

$\frac{1}{4}$

$S = \frac{3}{2} \quad L = 3$

for Fe $1s^2\ 2s^2 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^6$

$\Rightarrow Fe^{3+}$ ~~$1s^2\ 2s^2 2p^6\ 3s^2\ 3p^6$~~ $4s^2\ 3d^3$? ↑↓ ↑ ↑ ↑ — —

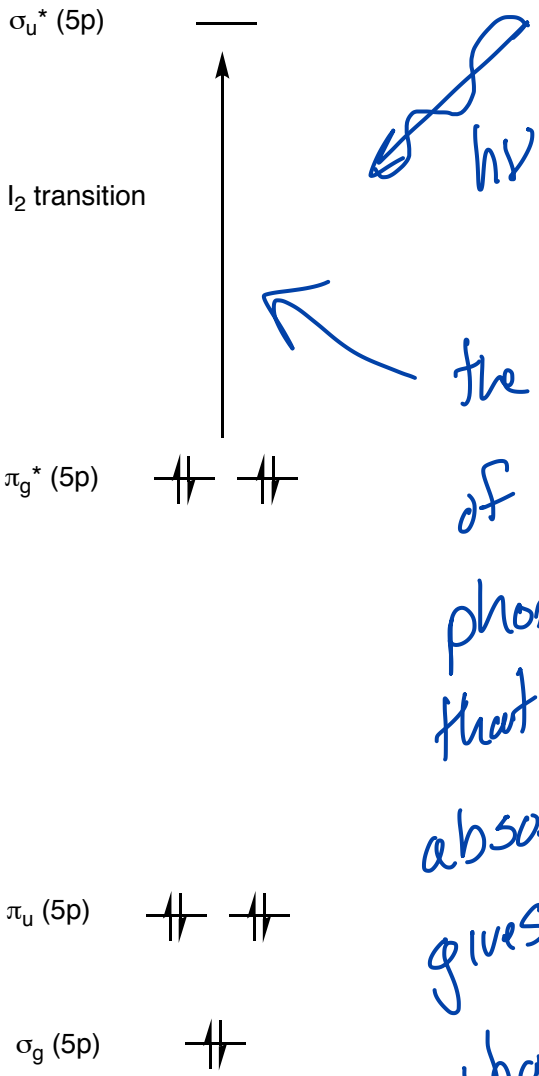
~~$1s^2\ 2s^2 2p^6\ 3s^2\ 3p^6$~~ $4s^0\ 3d^5$? this one

— ↑ ↑ ↑ ↑ ↑

$S = \frac{5}{2} \quad L = 0$

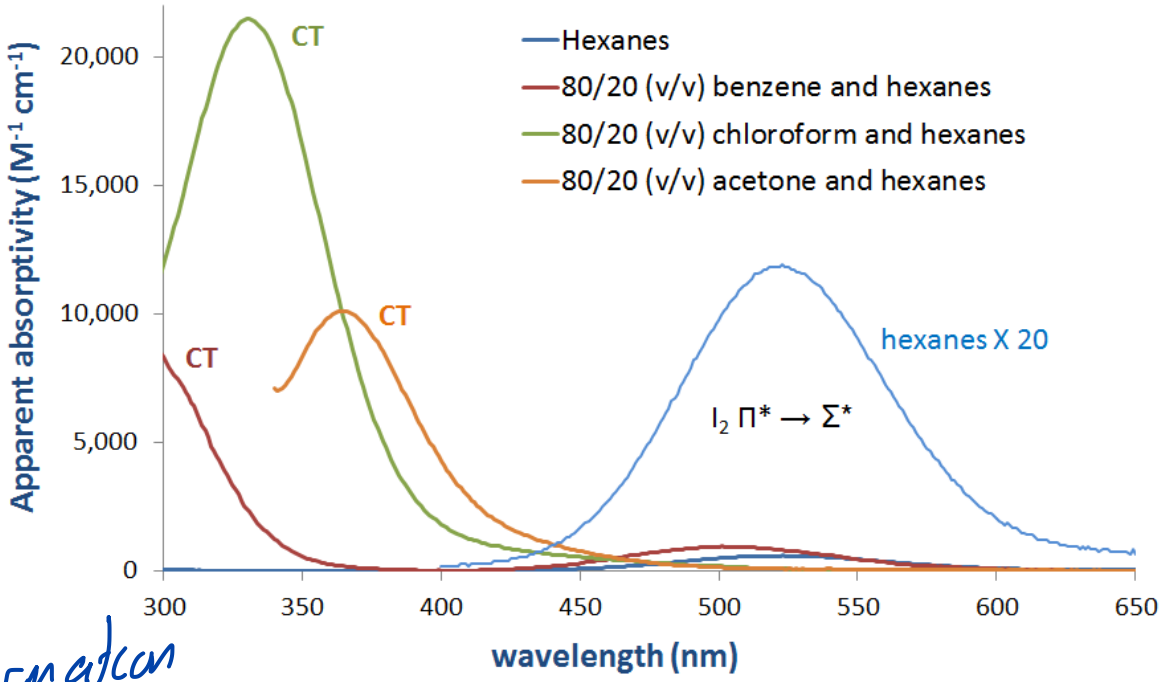
$\frac{1}{4}$

Magnetic susceptibility can help us answer this question



hν

the frequency of the photon that is absorbed gives us information about the gap between energy levels



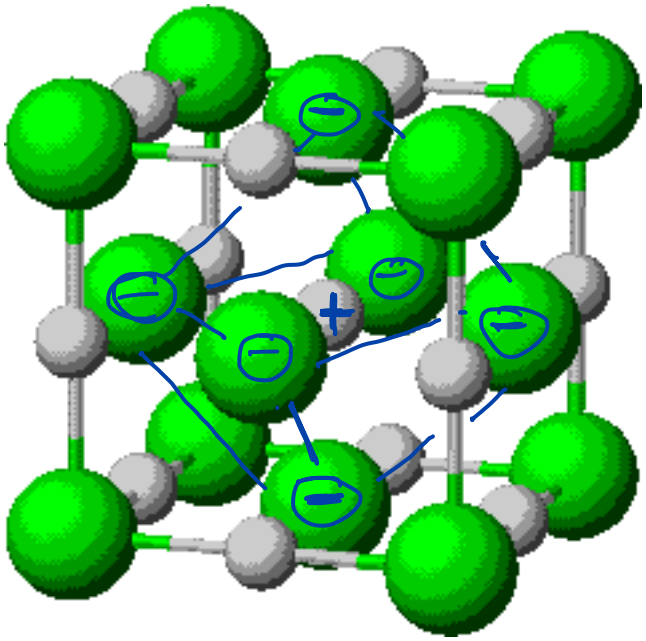
Crystal Field Theory

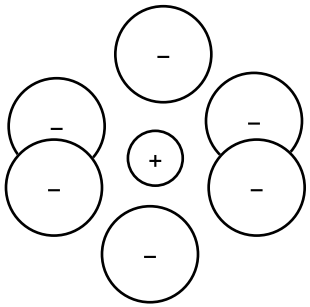
Electrostatic approach where d orbital splitting is explained using an ionic model

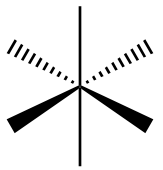
Ligand Field Theory

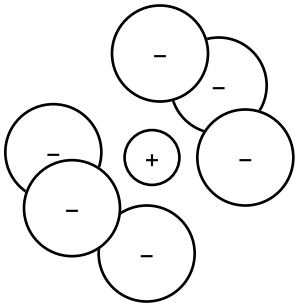
MO approach that describes bonding in terms of ligand HOMO/LUMO interactions with metal orbitals

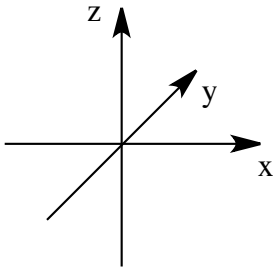
NaCl

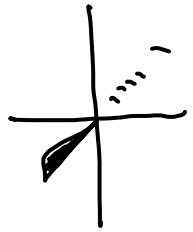




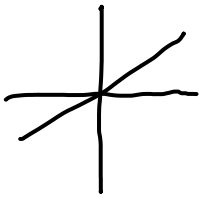








electron rich ligands interact with the metal at the center of the octahedron



Fe^{3+} ↑ ↑ ↑ ↑ ↑

spherical

octahedral field of e^-'s repels the d e^-'s differently

O_h Point Group

is used because the ligands are arranged in an octahedron

O_h	E	8 C_3	6 C_2	6 C_4	3 C_2 (C_4^2)	i	6 S_4	8 S_6	3 σ_h	6 σ_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		$(2z^2 - x^2 - y^2, x^2 - y^2)$
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, yz, xz)
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, x)	
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1		

d_{z^2}

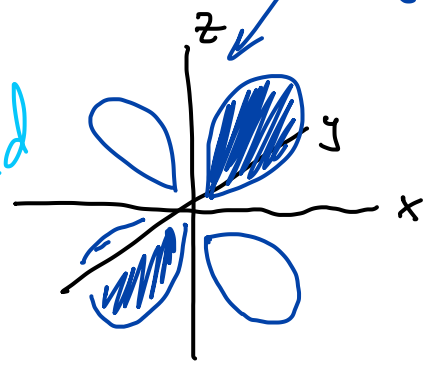
$d_{x^2 - y^2}$

d_{xy}, d_{yz}, d_{xz}

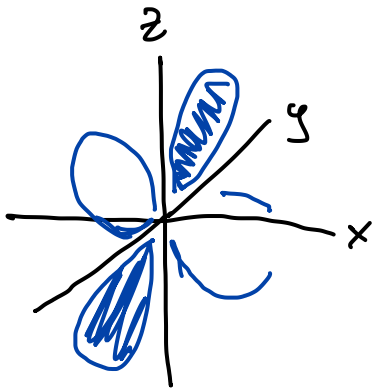
p_x, p_y, p_z

ligand e^-'s are inbetween the lobes of the orbitals

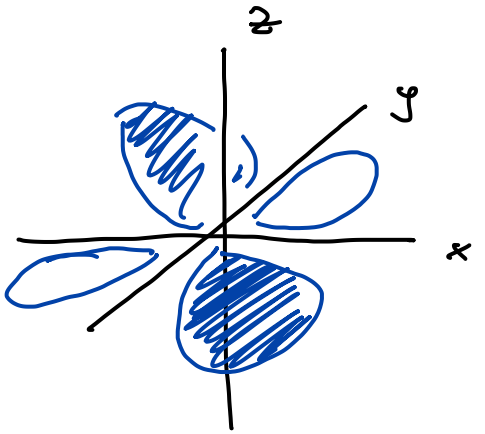
unchanged



d_{xz}



d_{yz}

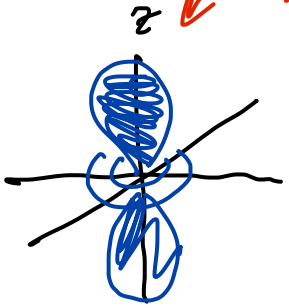


d_{xy}

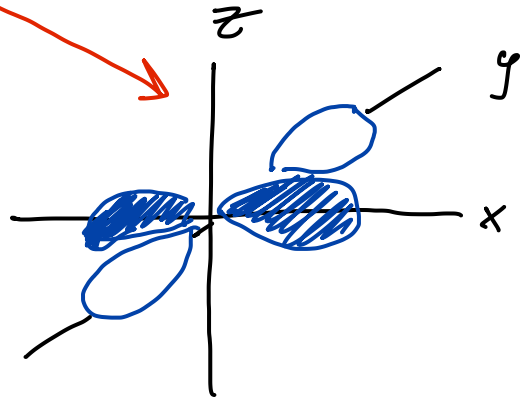
T_{2g}

increased in E

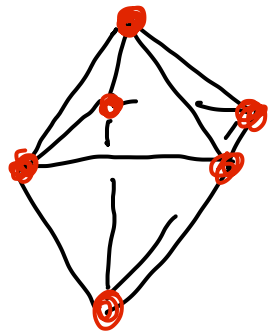
$e^- - e^-$ repulsion would increase E of this orbital



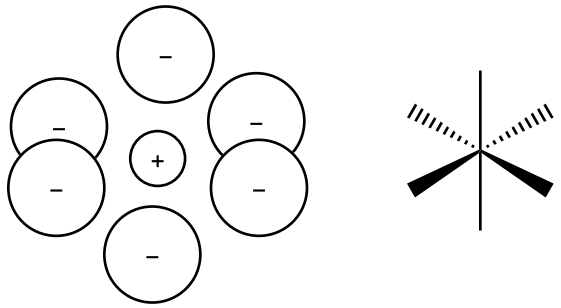
d_{z^2}

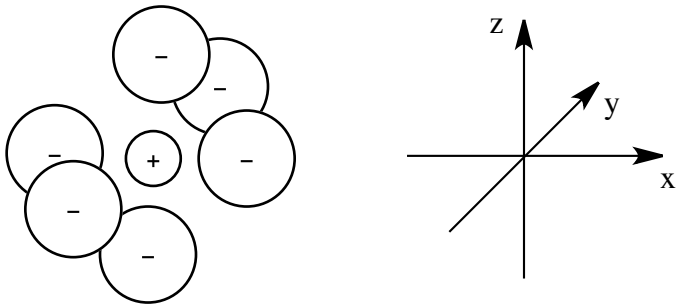


$d_{x^2-y^2}$



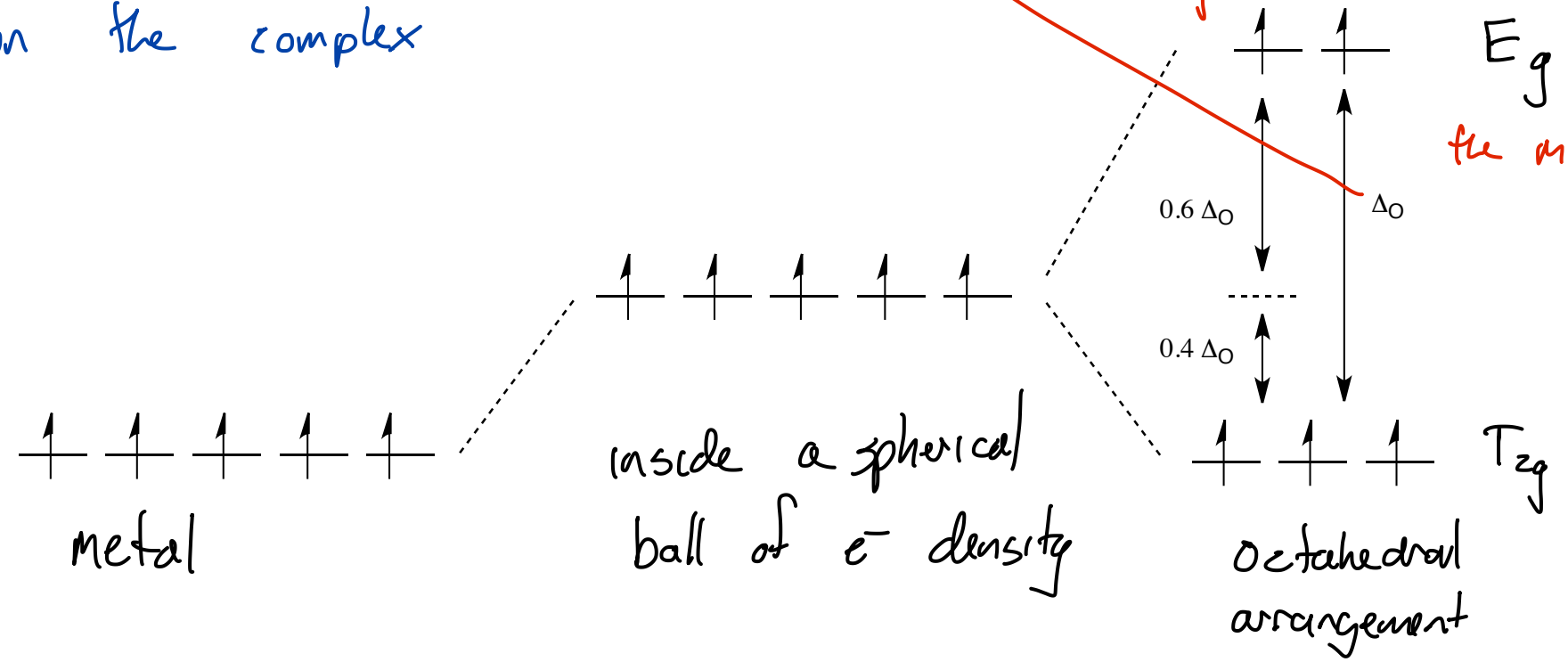
E_g



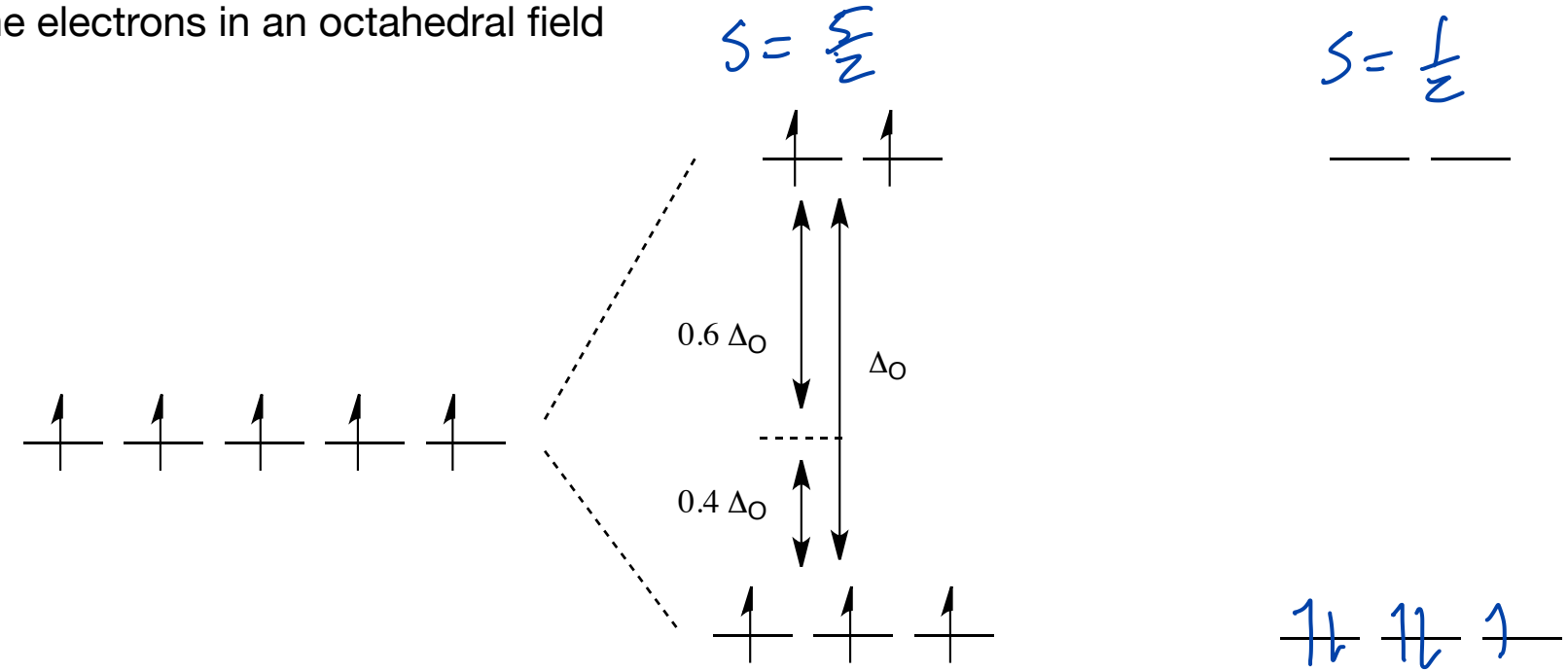


Δ_o = delta octahedral is a measure of how strongly the ligands interact with the metal

Find Δ_o how? shine photons on the complex



Crystal Field Stabilization Energy compares the energy of the electrons in a spherical field to the energy of the electrons in an octahedral field



CFSE = $E_{Octahedral}$ - $E_{spherical}$

$E_{spherical}$ = 0 + pairing energy

$E_{octahedral}$ = (# e^- x -0.4Δ_O) + (# e^- x 0.6Δ_O)

What will cause a molecule to be low spin?
What will make pairing e⁻'s more favorable than promoting e⁻?
The gap between T_{2g} & E_g ... big gap low spin small gap high spin
Strong e⁻ donors create larger gaps