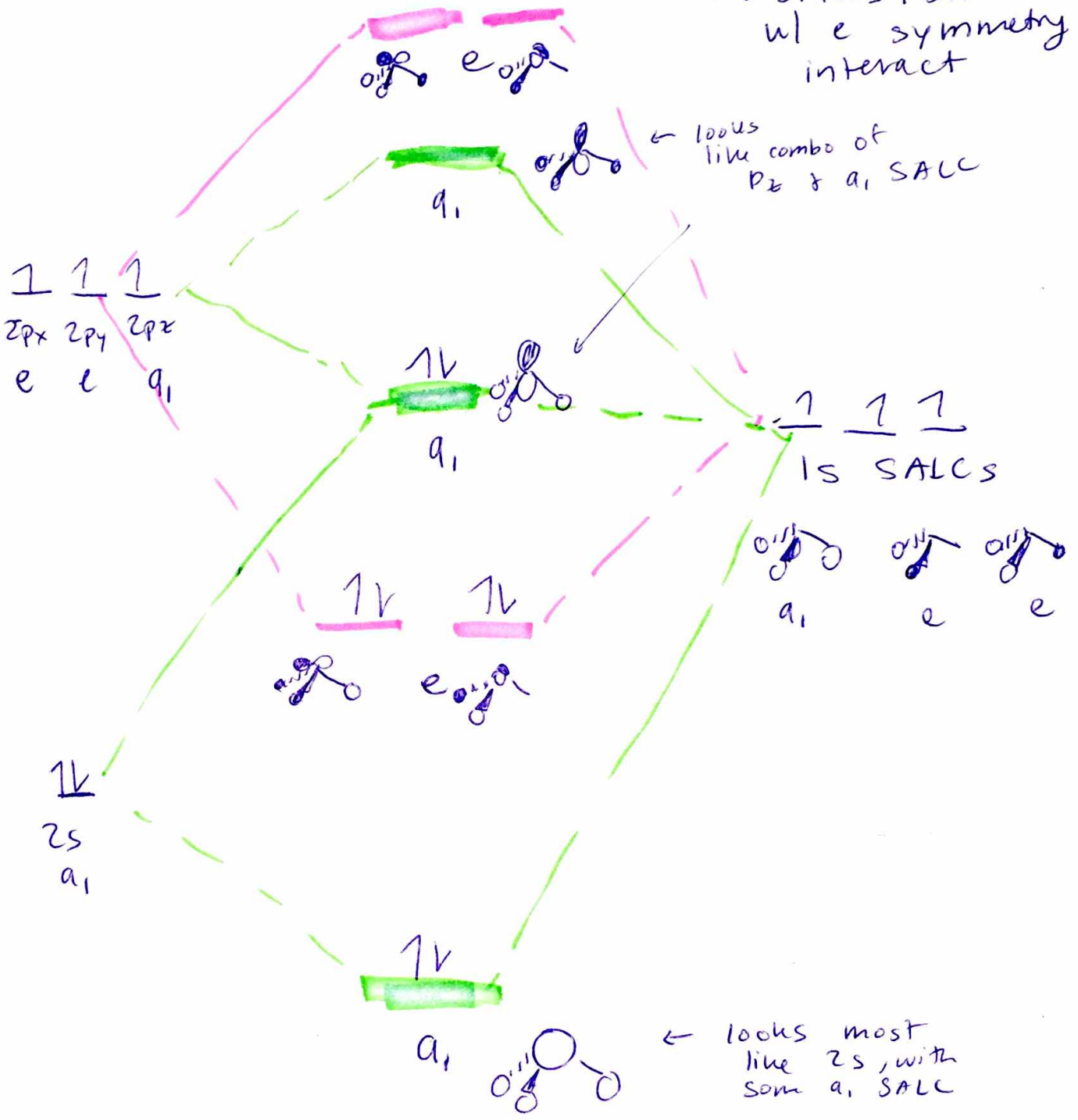
CH431 Lecture 14 10/13/16

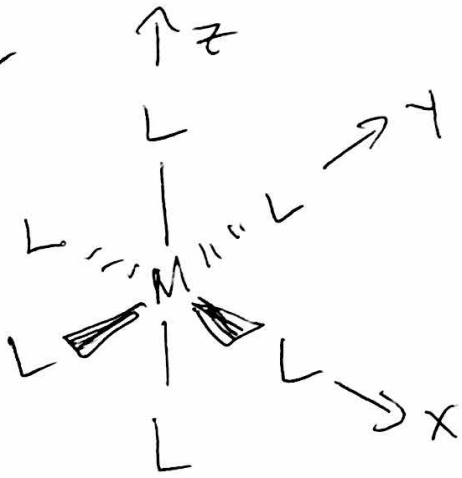
NH_3 MO diagram

- Orbitals / SALCs w/ a_1 symmetry interact
- orbitals / SALCs w/ e symmetry interact



Crystal Field theory

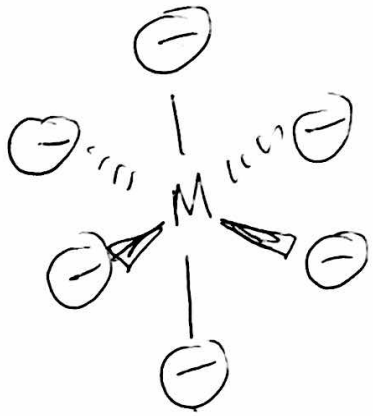
ML_6

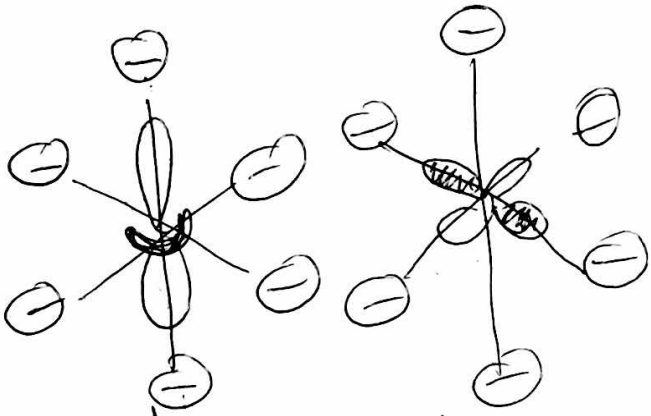


CFT

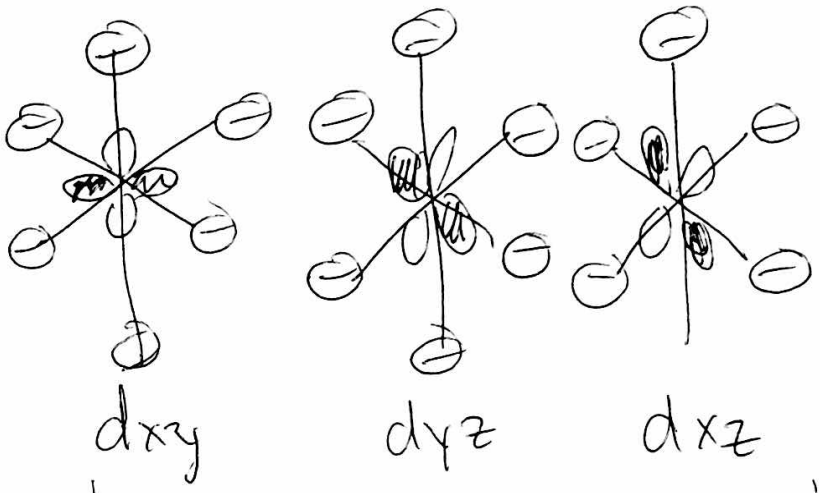
$\Rightarrow$

ligands are negative point charges

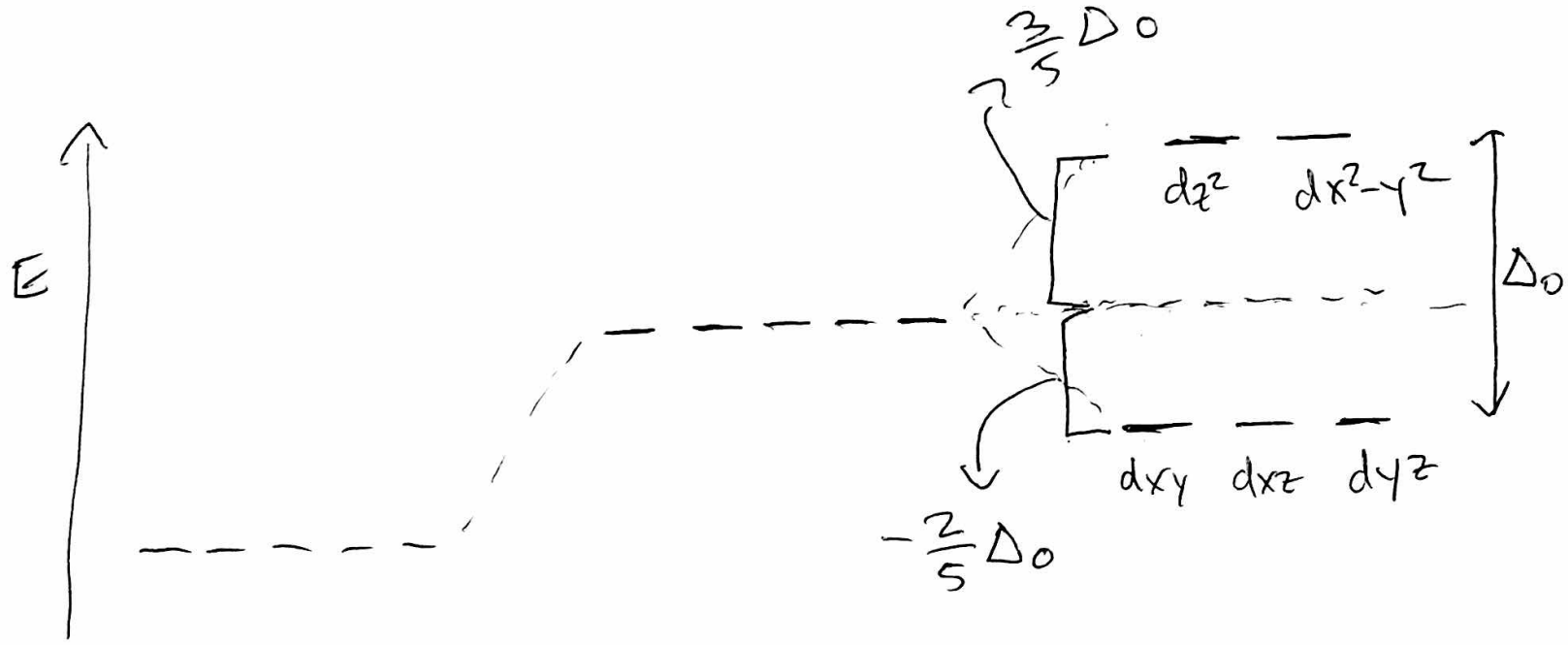




these orbitals will be destabilized due to repulsion between orbital and negative point charge



negative point charges do not align directly with orbitals, won't be destabilized as much



Free metal ion (no ligands)

Metal surrounded by a sphere of negative charge

Octahedral ML_6

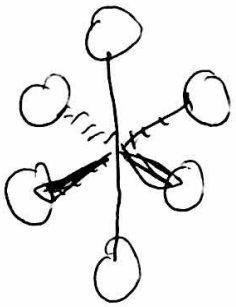
Δ_o: difference in energy between two d orbital energy levels

SALCs for sigma-only ML_6

$\Gamma_s = A_{1g} + T_{1u} + E_g$

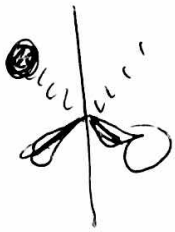
$\downarrow$ $\downarrow$ $\downarrow$

s p_x, p_y, p_z $d_{z^2}, d_{x^2-y^2}$



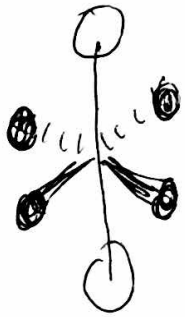
a_{1g}

t_{1u} (p_z)

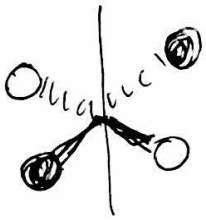


t_{1u} (p_x)

t_{1u} (p_y)

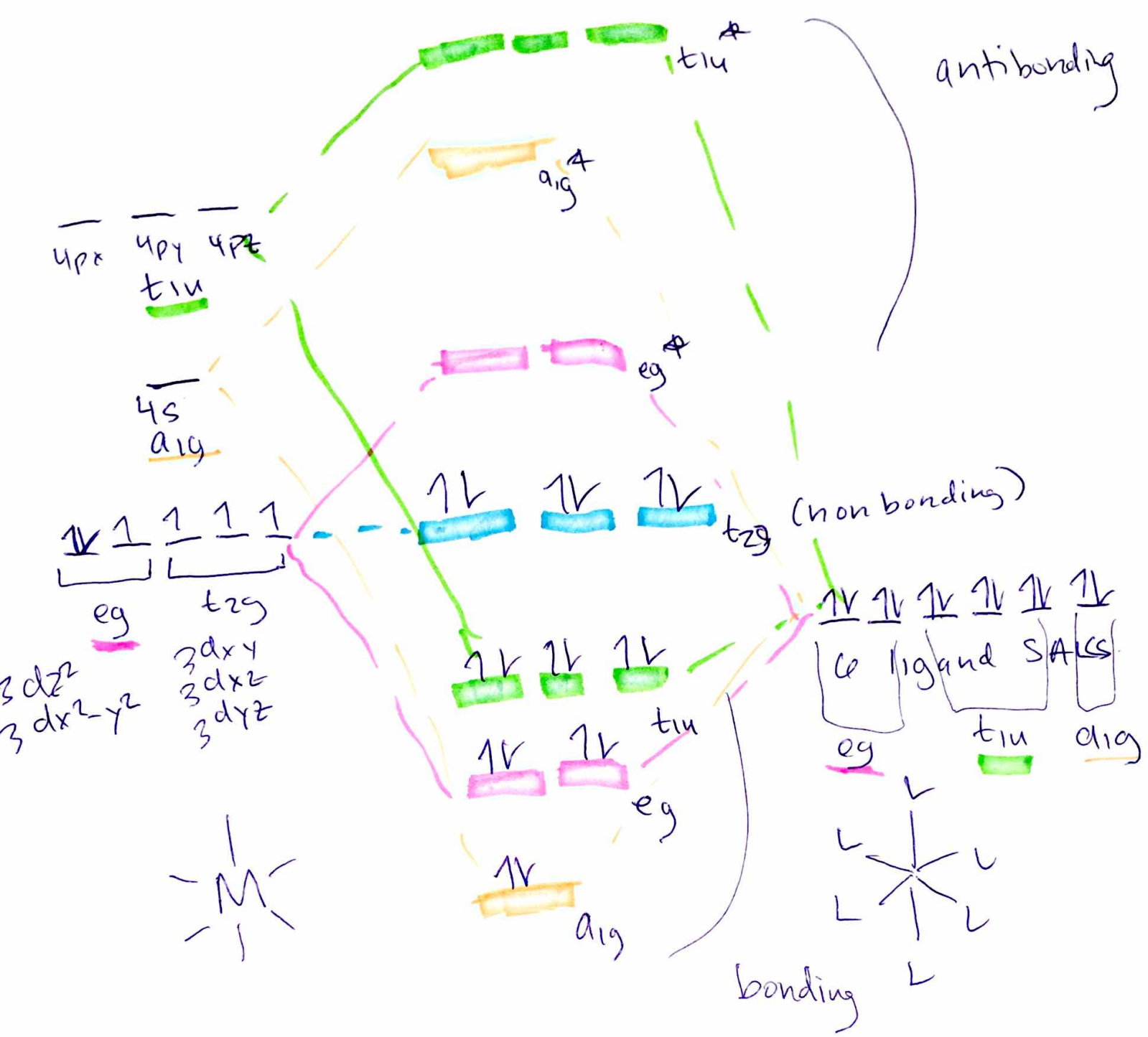


e_g d_{z^2}



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

MO treatment to determine d orbital splitting


t1u*
antibonding
a1g*
4px 4py 4pz
t1u
eg*
4s
a1g
(nonbonding)
t2g
eg
t2g
3dz2
3dx2-y2
3dxy
3dxz
3dyz
t1u
eg
a1g
M
L
bonding
Fe2+ d6
2 electrons from each ligand → 12 total