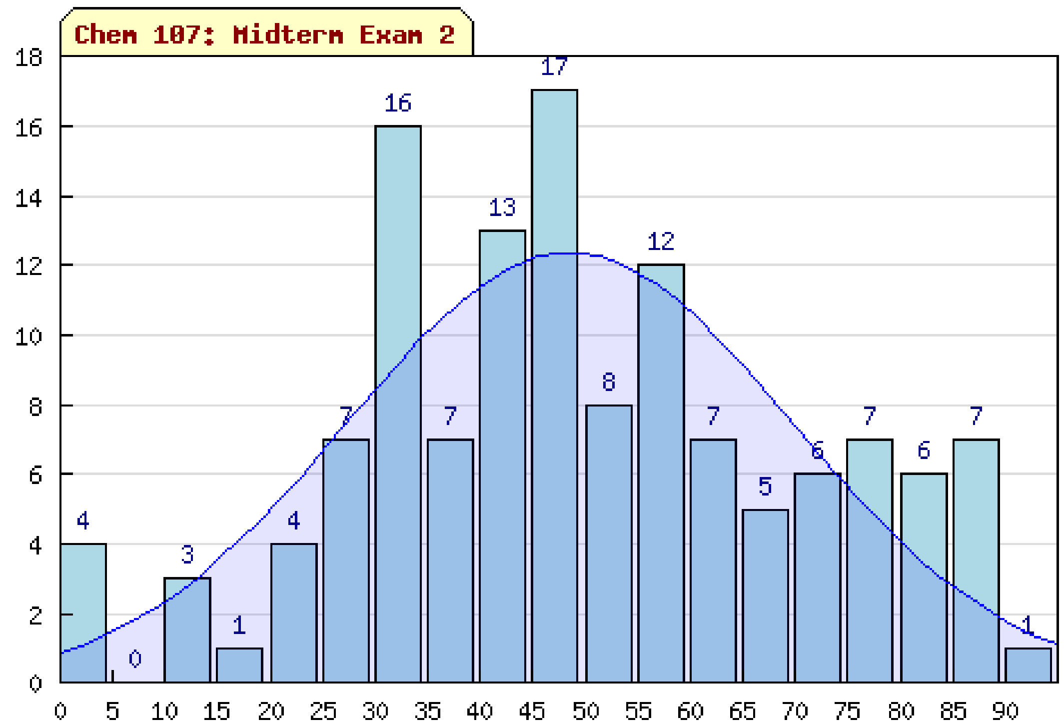
Coordination Chemistry II: Ligand Field Theory

Chapter 10

Monday, November 23, 2015

Midterm II Results



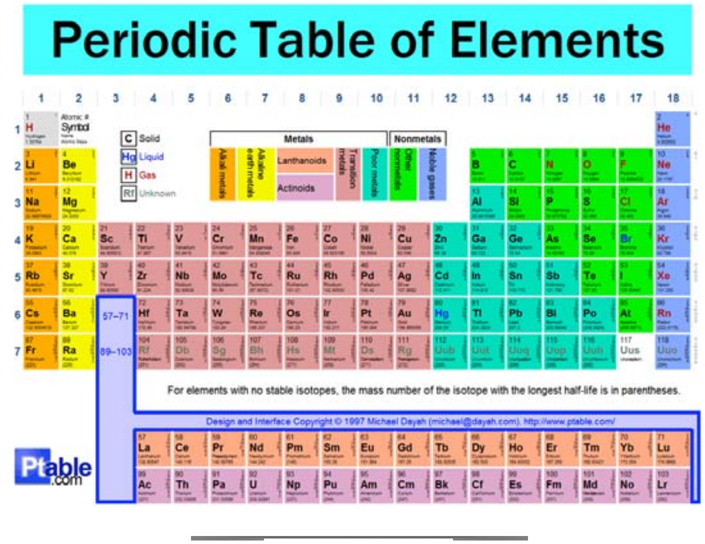
Mean: 49 (out of 85 pts; 58% - increased by 23% from exam 1)
Median: 48
Mode: 45
Max: 93
Min: 0
SD: 21

Ligand Field Theory

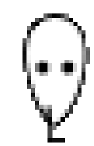
In LFT we use metal valence orbitals and ligand frontier orbitals to make metal–ligand molecular orbitals

Metal valence orbitals:

Sc – Zn	*3d*	*4s*	*4p*
Y – Cd	*4d*	*5s*	*5p*
La – Hg	*5d*	*6s*	*6p*



Ligand frontier orbital:



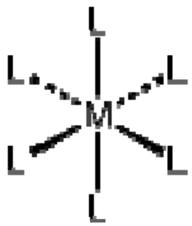
For now we will only consider σ-bonding with the ligands

***O*$_h$ first!**

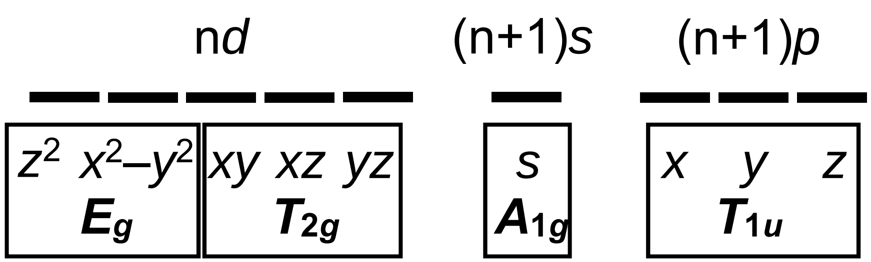
We already did this: see 10/18 lecture.

σ-MOs for Octahedral Complexes

We use group theory to understand how metal and σ-ligand orbitals interact in a complex:

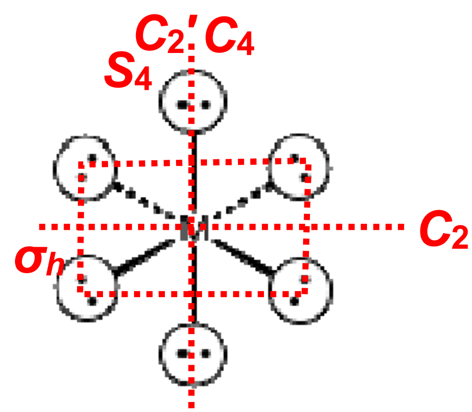


O_h



symmetries (irr. reps.) of the metal valence orbitals are obtained directly from the character table

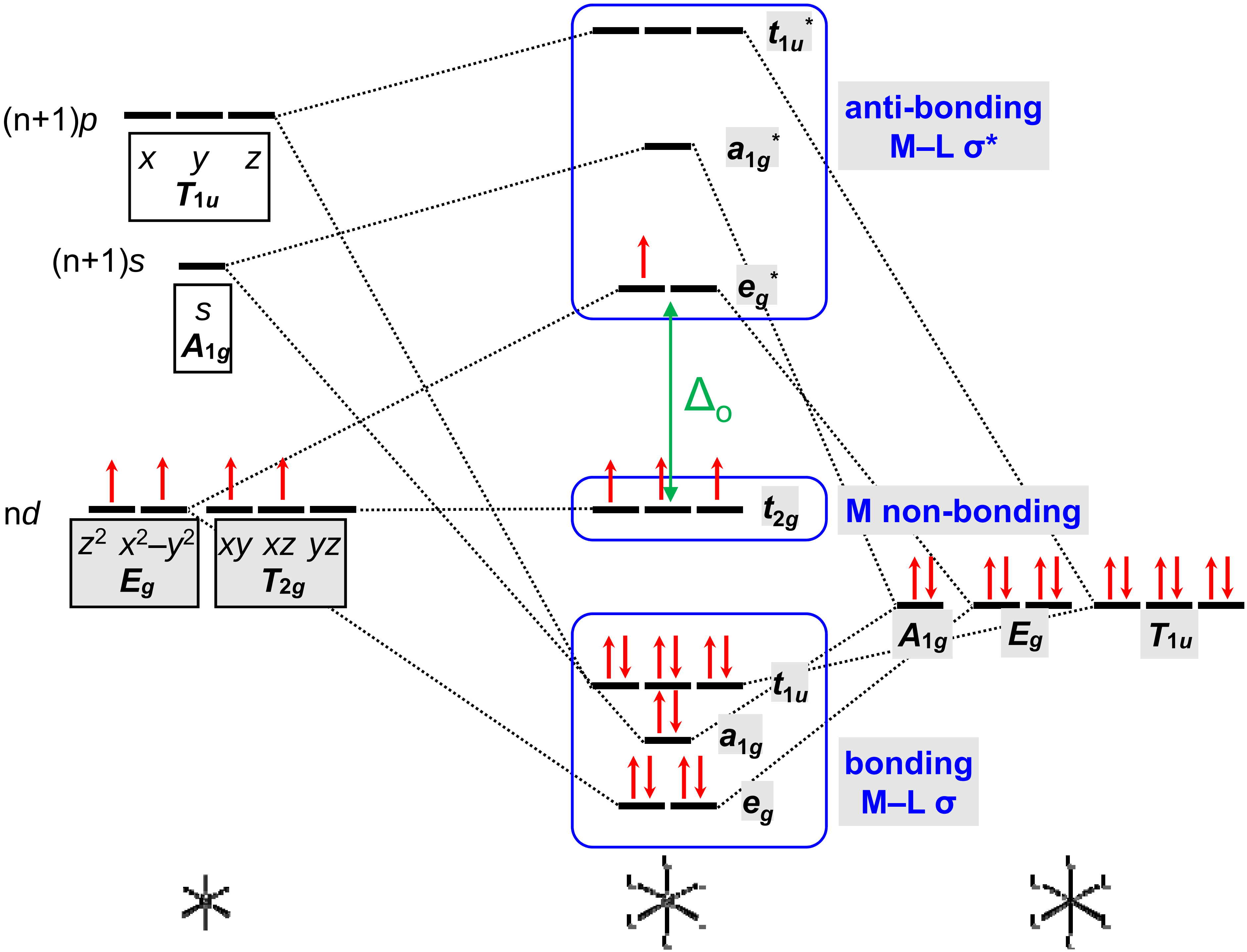
We need to determine the reducible representation for the σ-ligand orbitals in O_h:



the total ligand representation (Γ_σ) can be decomposed as we learned in 4.4.2

	E	$8C_3$	$6C_2$	$6C_4$	$3C_2'$	i	$6S_4$	$8S_6$	$3\sigma_h$	$6\sigma_d$	irreducible representations
Γ_σ	6	0	0	2	2	0	0	0	4	2	$A_{1g} + E_g + T_{1u}$

σ-ML_6 Octahedral MO Diagram



MO Pictures

It is also helpful to visualize the MOs so we understand the electron distribution within a coordination complex