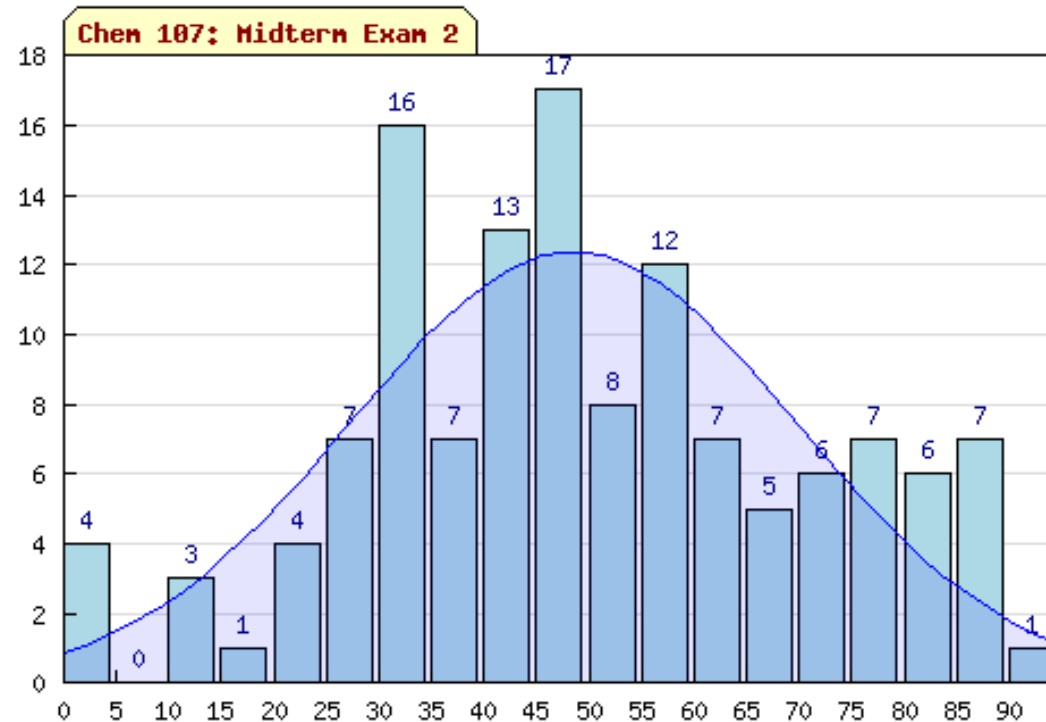


Coordination Chemistry II: Ligand Field Theory

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

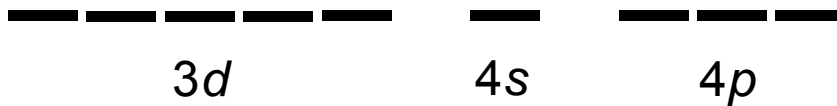
SD: 21

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



Y – Cd



La – Hg



Periodic Table of Elements

A standard periodic table of elements with color-coded groups. The groups are labeled: Alkali metals, Alkaline earth metals, Transition metals, Lanthanoids, Actinoids, Post-transition metals, Nonmetals, and Noble gases. The table includes atomic number, symbol, and name for each element. A note at the bottom states: "For elements with no stable isotopes, the mass number of the isotope with the longest half-life is in parentheses." The source is cited as "Design and Interface Copyright © 1997 Michael Dayeh (micheel@dayeh.com), http://www.ptable.com/".

Ligand frontier orbital:



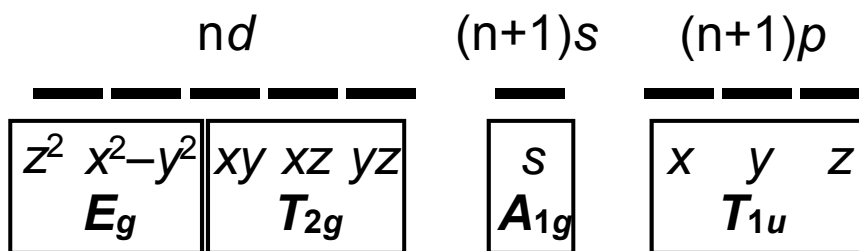
For now we will only consider σ -bonding with the ligands

O_h first!

We already did this: see 10/18 lecture.

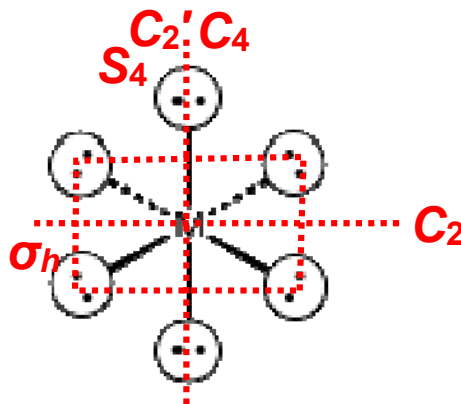
σ -MOs for Octahedral Complexes

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



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

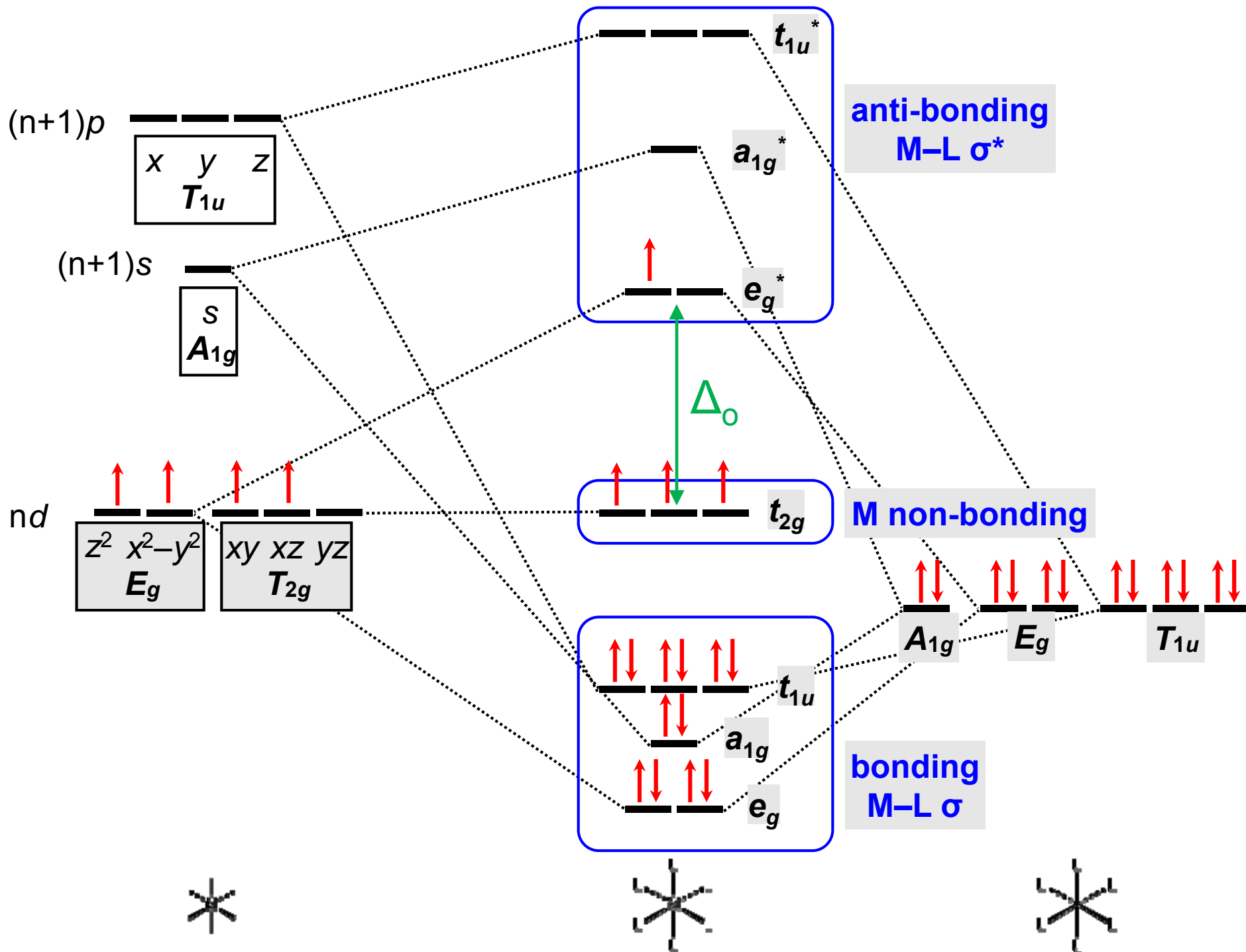
We need to determine the reducible representation for the σ -ligand orbitals in O_h :



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 -ML₆ Octahedral MO Diagram



MO Pictures

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

