Chem 111

Lecture 20

Announcements

- Exam 2, Nov 1

→Pencils, Erasers, Calculator, ID card

- Practice Exams:

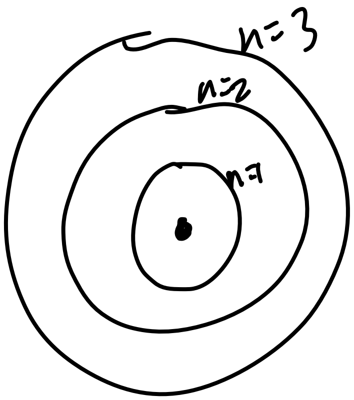
http://courses.umass.edu/chem111-bbotch/ExamInfo.html

- Breanne has a recitation session HASA 126 – 10/27 (5-6pm)

- SI session schedule is posted on website

Recap

- Bohr Model



Let's Practice

$$\frac{hc}{\lambda} = h\nu = \Delta E = R_H hc\left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

Calculate the wavelength of light that corresponds to the transition of the electron ~~form~~ from the n=4 to the n=2 state of the hydrogen atom. Is the light absorbed or emitted?

$$\frac{1}{\lambda} = R_H \left(\frac{1}{n_i^2} - \frac{1}{n_f^2}\right)$$

$$= (1.097 \times 10^7\ m^{-1})\left(\frac{1}{4^2} - \frac{1}{2^2}\right)$$

$$\lambda = -4.86 \times 10^{-7}\ m$$

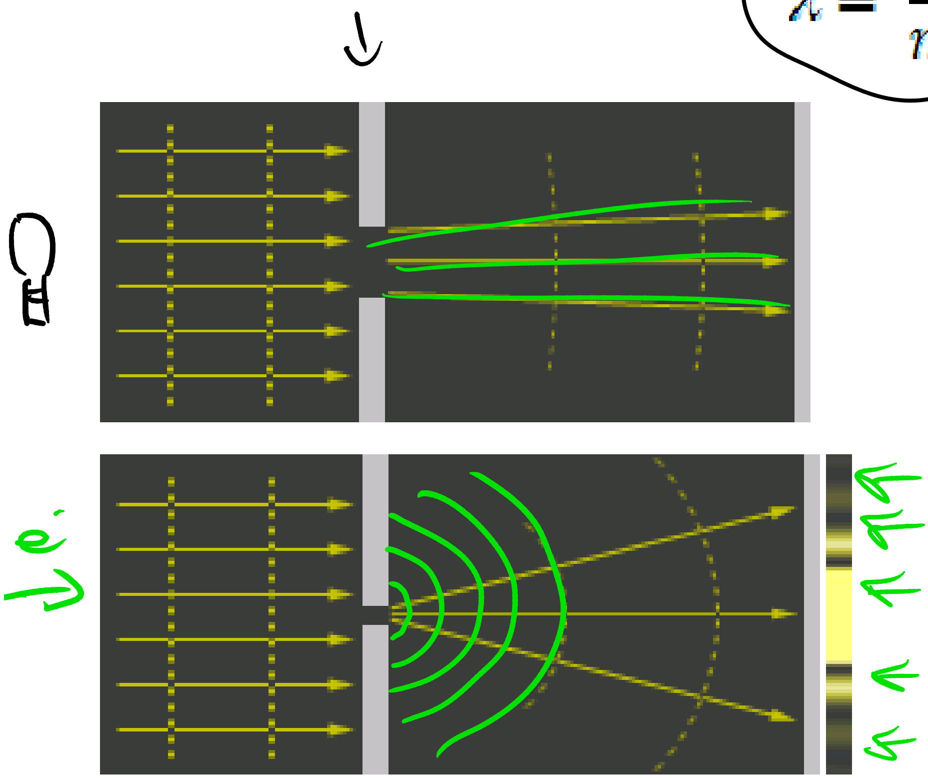
486 nm

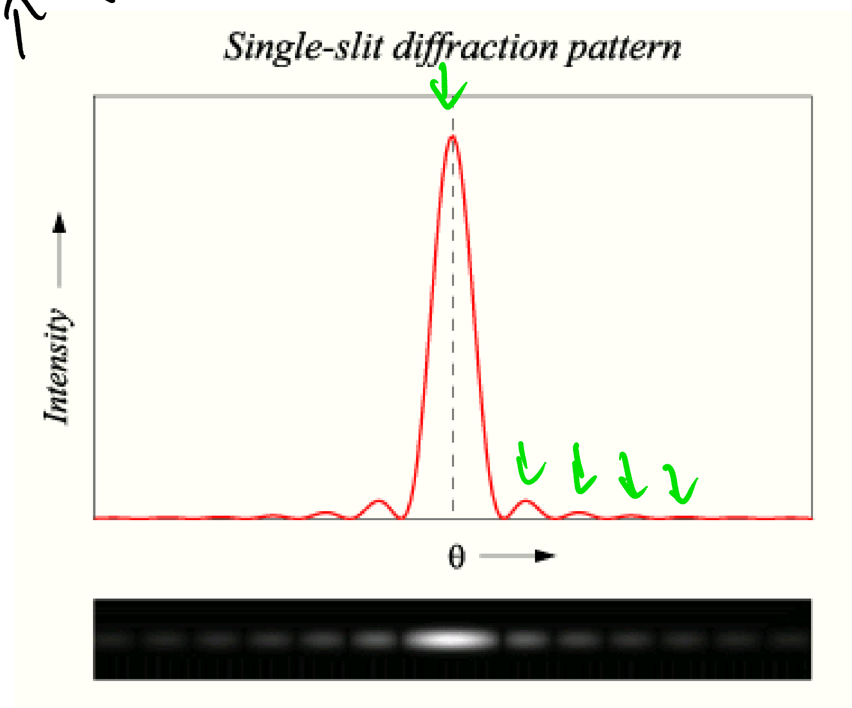
Wave-Particle Duality

Light has wave and particle like characteristics.
What about something that mass.

$$\lambda = \frac{h}{mv}$$

v = velocity
m = mass

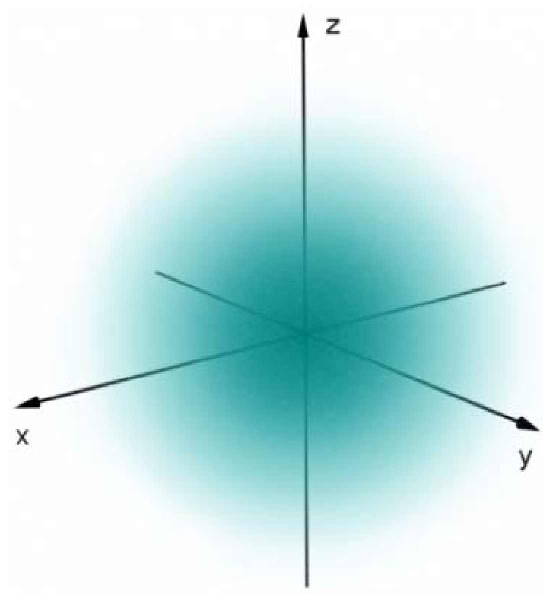




Quantum Mechanics

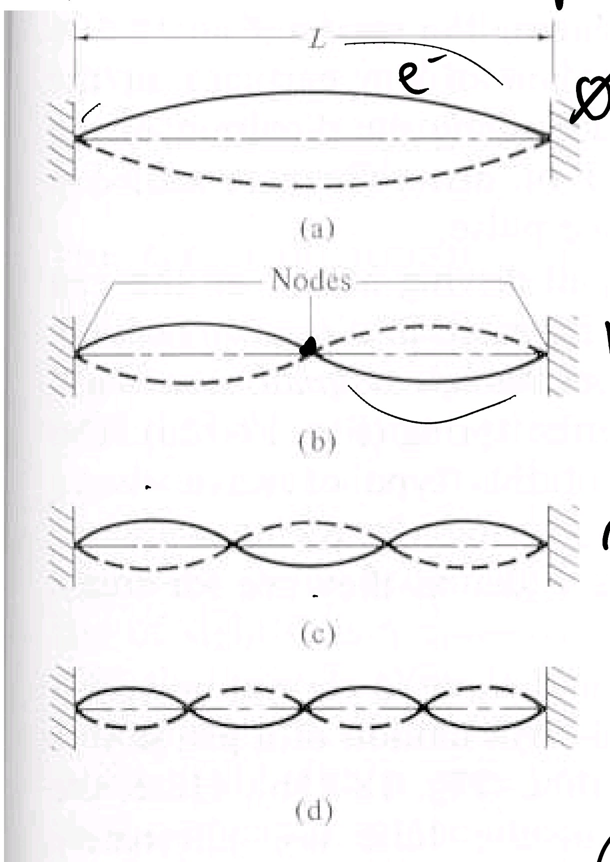
Uncertainty Principle: It is impossible for us to simultaneously both the exact momentum of the electron and its exact location in space.

Schrödinger's equation: Incorporates wave like and particle behavior. Through these we are able to calculate probabilities of where the electron location.

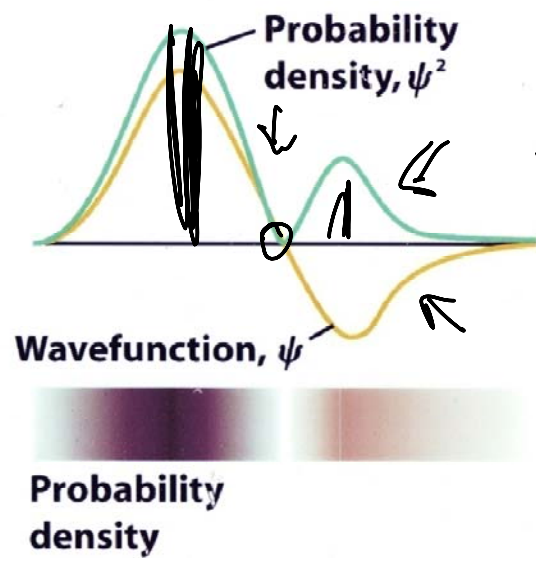


Schrödinger's Equation

- Treat the electron as a standing wave.

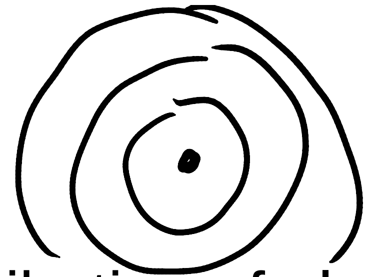


When the amplitude passes zero, we call that a **node**.



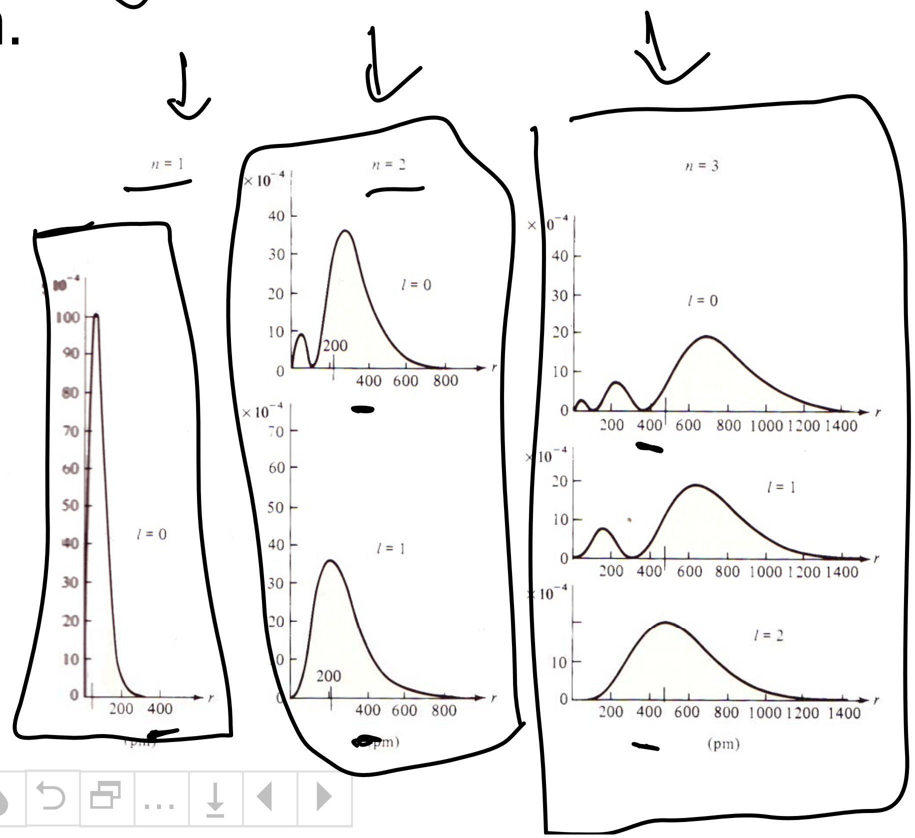
High probabilities makes orbitals

Quantum Numbers



- Each **orbital** describes a specific distribution of electron density in space, given by its probability density.

- The principle quantum number, n, can have integral value of 1, 2, 3 and so forth.



- As n increases the electron spends more time away from the nucleus (has a higher energy).

- Electron shell

Quantum Numbers

- The Azimuthal quantum number, ℓ, can be integral values of 1 to n-1.
- This describes the shape of the orbital.
- Sometimes letter are used instead of numbers. 0=s; 1=p; 2=d; 3=f
- Subshell

Quantum Numbers

m_ℓ

- The magnetic quantum number, m_ℓ, can have intergral values between $-\ell$ and ℓ, including zero. $\ell = 1$

  $m_\ell = -1, 0, 1$

- The quantum number describes the orientation of the orbital in space.

Quantum Numbers

TABLE 6.1 Summary of the Quantum Numbers, Their Interrelationships, and the Orbital Information Conveyed

Principal Quantum Number	Azimuthal Quantum Number	Magnetic Quantum Number	Number and Type of Orbitals in the Subshell
Symbol = n Values = 1, 2, 3, . . . n = number of subshells	Symbol = ℓ Values = 0 . . . $n - 1$	Symbol = m_ℓ Values = $+\ell$ . . . 0 . . . $-\ell$	Number of orbitals in shell = n^2 and number of orbitals in subshell = $2\ell + 1$
1	0	0	one 1*s* orbital (one orbital of one type in the $n = 1$ shell)
2	0 1	0 +1, 0, −1	one 2*s* orbital three 2*p* orbitals (four orbitals of two types in the $n = 2$ shell)
3	0 1 2	0 +1, 0, −1 +2, +1, 0, −1, −2	one 3*s* orbital three 3*p* orbitals five 3*d* orbitals (nine orbitals of three types in the $n = 3$ shell)
4	0 1 2 3	0 +1, 0, −1 +2, +1, 0, −1, −2 +3, +2, +1, 0, −1, −2, −3	one 4*s* orbital three 4*p* orbitals five 4*d* orbitals seven 4*f* orbitals (16 orbitals of four types in the $n = 4$ shell)

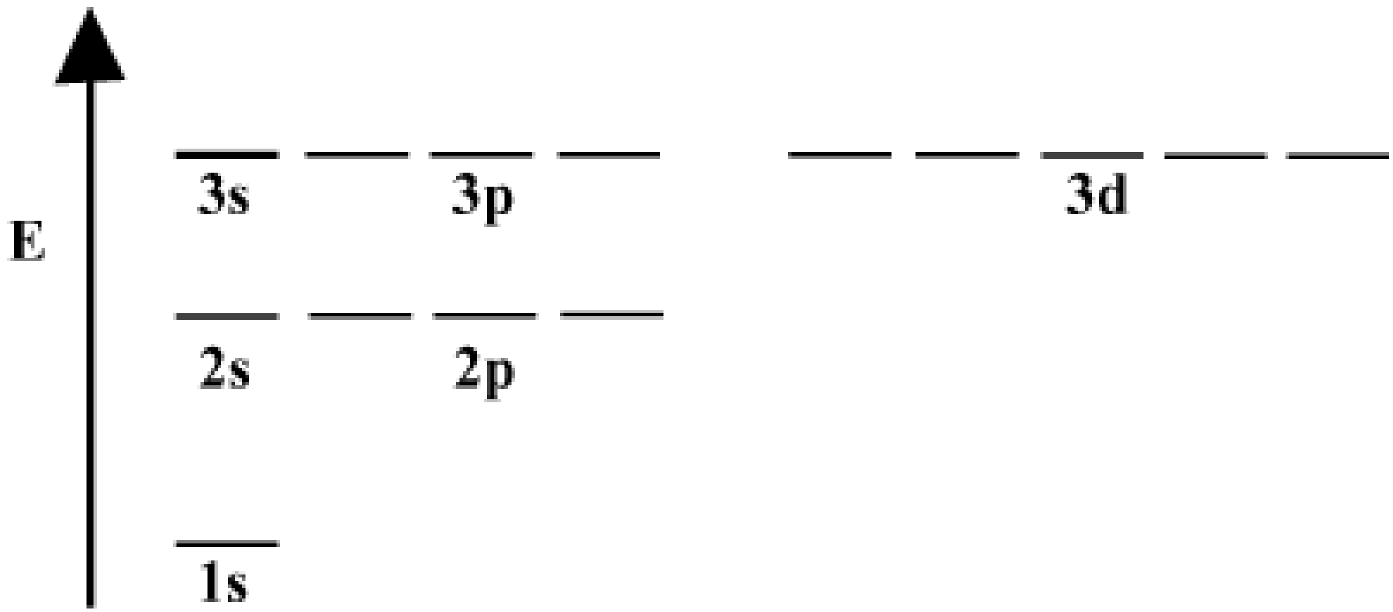
Quantum Numbers

- The shell with principle quantum number n will consist of exactly n subshells.

- For a given value of ℓ, there are $2\ell + 1$ values of m_ℓ.

- The total number of orbitals in a shell is n^2

Orbitals



s-orbital

n = 1
n = 2
n = 3
l = 0

- # nodal planes = l

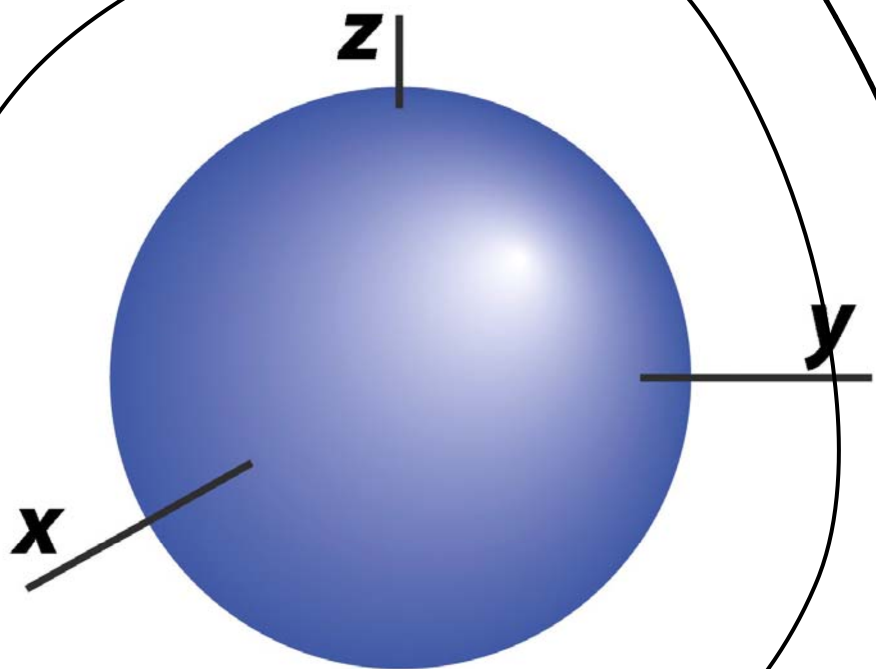


Figure 1-15
Shriver & Atkins Inorganic Chemistry, Fourth Edition

p-orbitals

$l = 1$

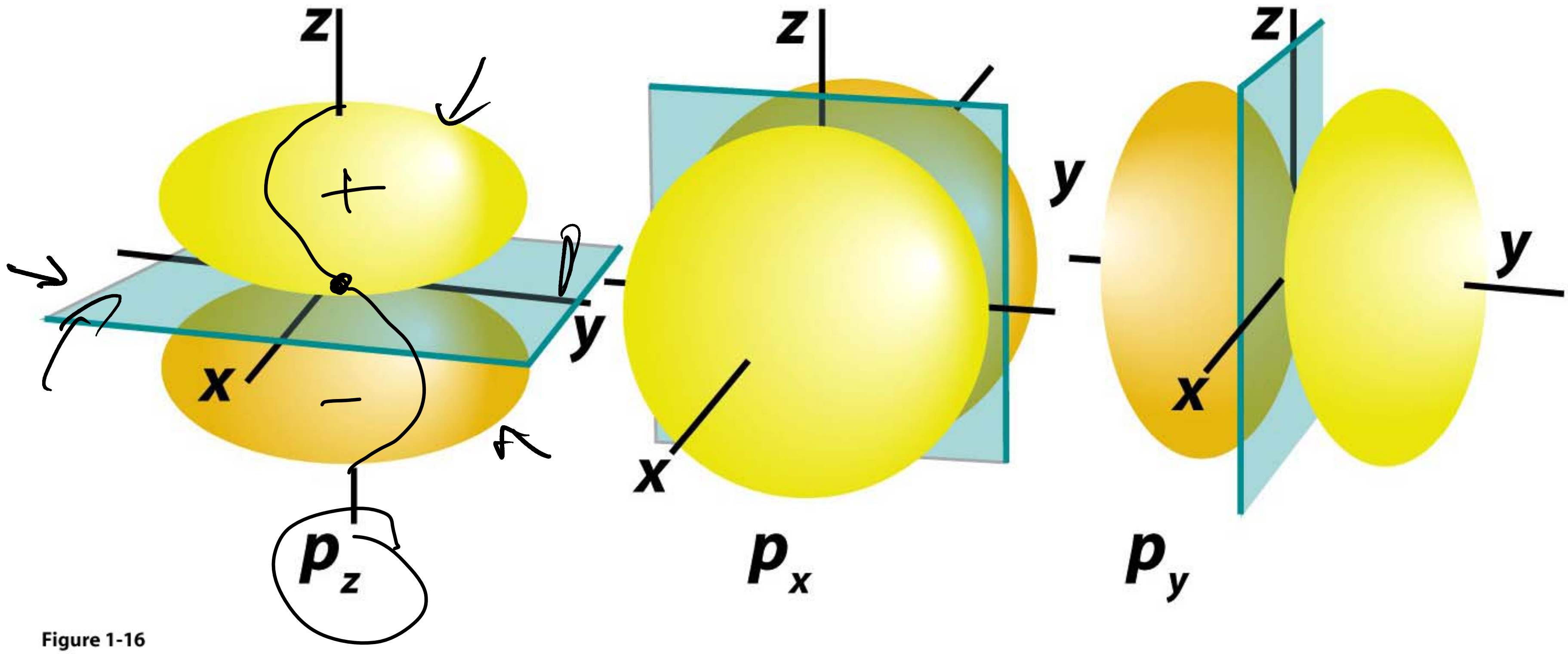
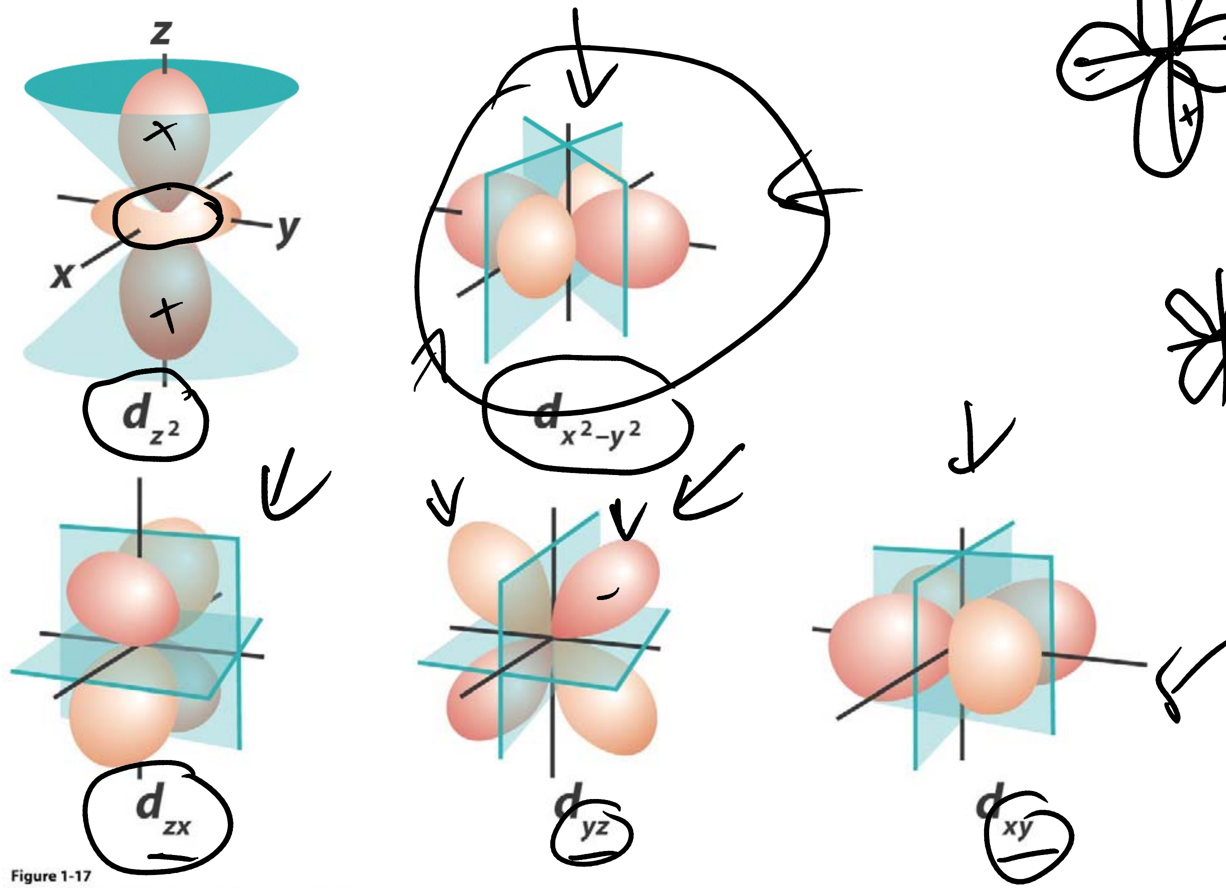


Figure 1-16
Shriver & Atkins Inorganic Chemistry, Fourth Edition

d-orbitals

$l = 2$



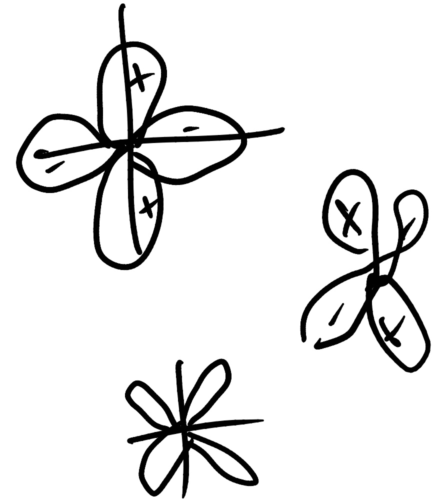


Figure 1-17
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f-orbitals

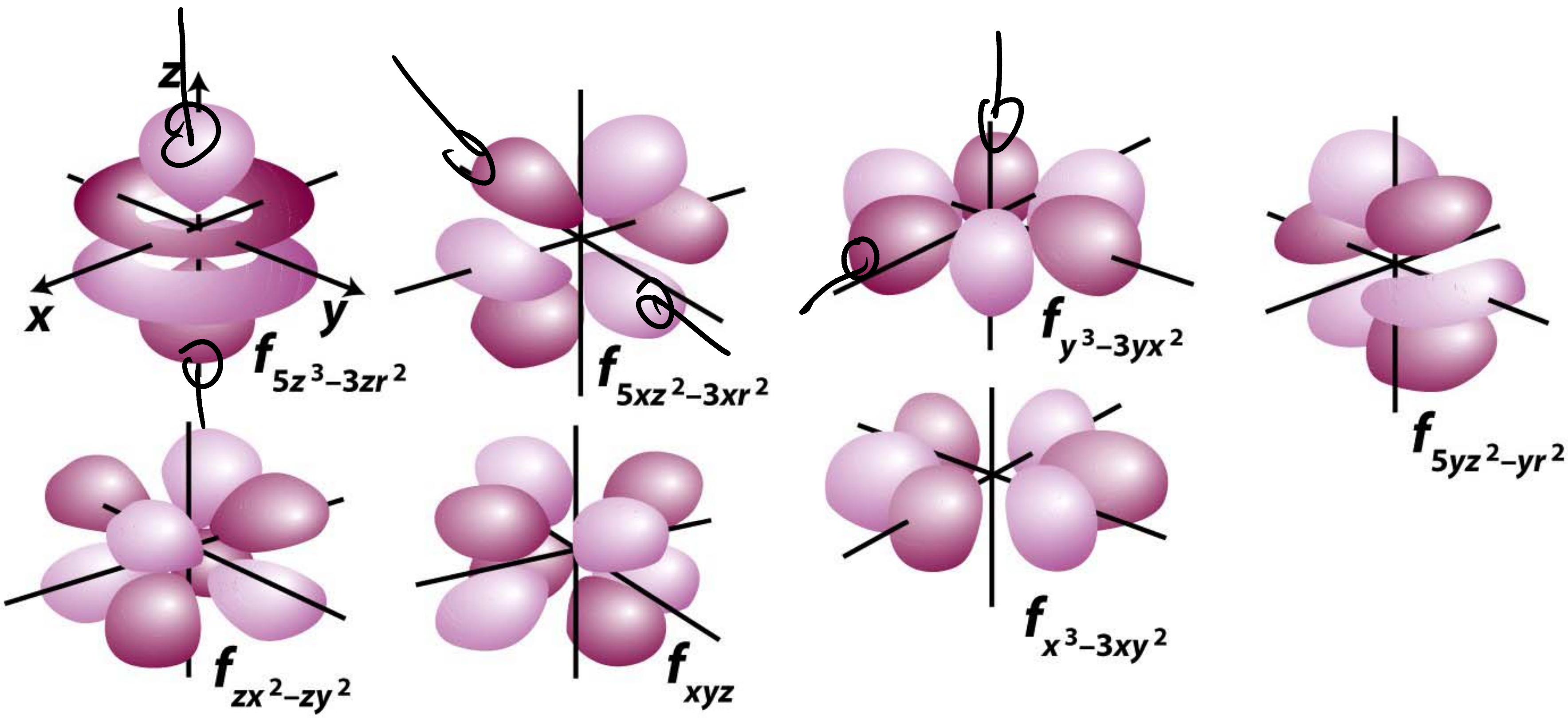
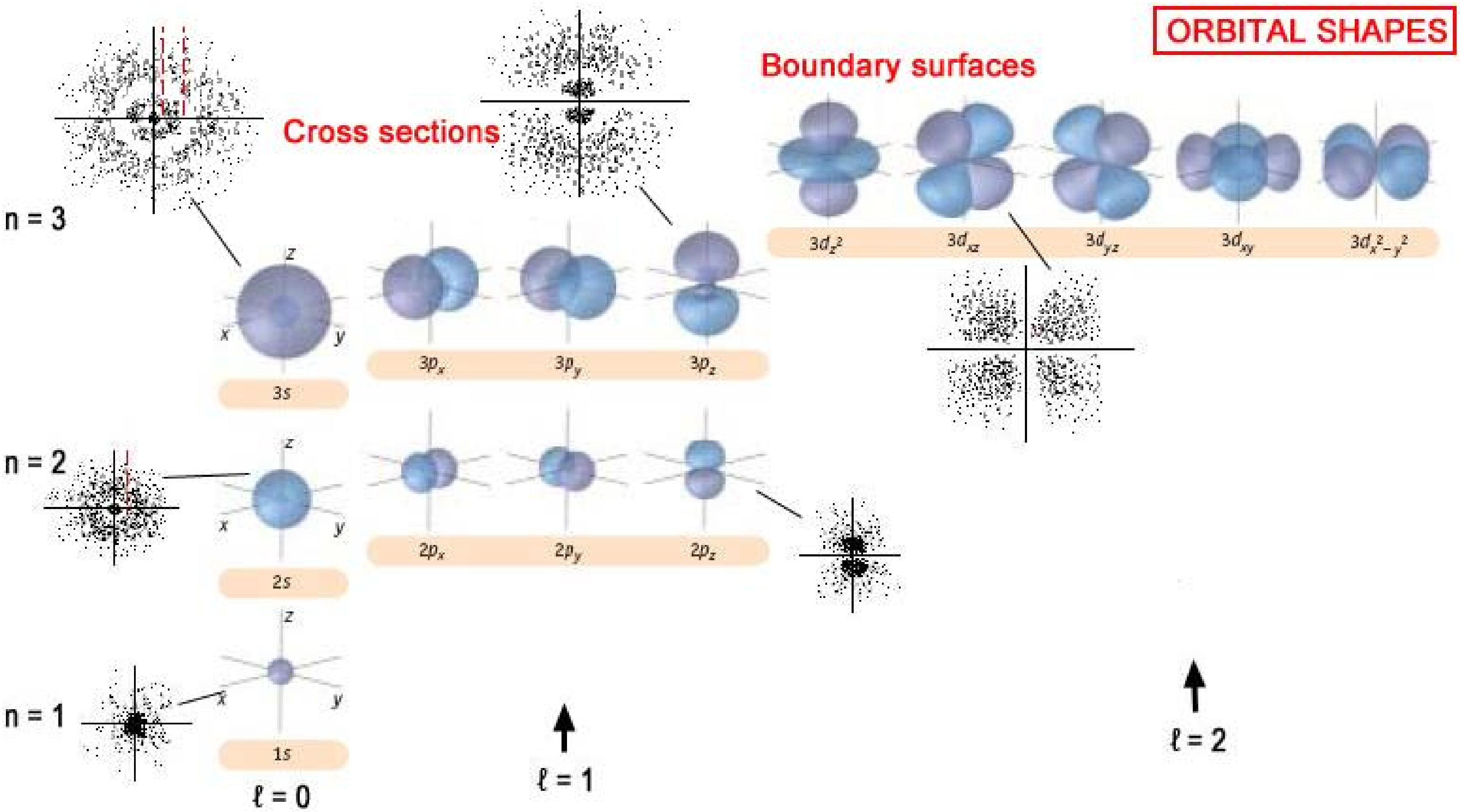


Figure 1-18
Shriver & Atkins Inorganic Chemistry, Fourth Edition

Q#



ORBITAL SHAPES
Boundary surfaces
Cross sections
n = 3
n = 2
n = 1
3s
3px
3py
3pz
2s
2px
2py
2pz
1s
3dz2
3dxz
3dyz
3dxy
3dx2−y2
ℓ = 0
ℓ = 1
ℓ = 2

Spin

- s = intrinsic angular spin.
- For an electron s=1/2 always
- m_s = spin magnetic q#
- For and electron m_s = +1/2 or -1/2

The for q# n, l, m_l, m_s are used to characterize a electron in an atom