(4) Today
2.2.2 Quantum Numbers and Atomic Wave Functions
2.2.3 The Aufbau Principle
2.2.4 Shielding
(6) Second Class from Today
2.3 Periodic Properties
3.1 Lewis Structures
3.2 VSEPR

Third Class from Today (7)
3.2 VSEPR

Orbitals and Quantum Numbers ( $\mathrm{n}, \mathrm{l}$, and $\mathrm{m}_{\mathrm{I}}$ )

One quantum number wasn't enough to model the electrons in an atom $n$ is the principal quantum number
allowed values are the whole numbers starting a 1
I is the Angular momentum quantum number

$$
e^{-} \quad n=1 \quad l=0 \quad \sum \geq x
$$

allowed values are the from $n$ to 0 in whole number increments $e^{-} \quad n=2 \quad l=0$
$m_{l}$ is the magnetic quantum number

$$
n=2 \quad l=1
$$

allowed values are the from $-l$ to $/$ in whole number increments

$$
n=1 \quad l=0 \quad m_{l}=0
$$

$\mathrm{m}_{\mathrm{s}}$ is the spin quantum number

$$
\begin{aligned}
& \text { allowed values are }-1 / 2 \text { or }+1 / 2 \\
& e^{-} \quad n=2 \quad l=1 \quad m_{l}=0 \quad m_{s}=+\frac{1}{2} \\
& 2 p e^{-} \\
& \ell=0 \quad 5 \\
& l=1 \quad p \\
& l=2 d \\
& l=3 \quad f \\
& \text { values } \\
& \text { priazipal orbital } 3 \text { orbitalswith } \\
& \text { enogy type } l=1 \text { shape } \\
& \text { level } \\
& \text { in def direct- } \\
& \text { rods }{ }^{2}
\end{aligned}
$$

## The angular distribution function:

The square of the angular distribution function describes the probability of finding the electron at angles $\theta$ and $\phi$. In other words, picture yourself standing on the nucleus, and the electrons look like fog around you. The square of the angular distribution function describes how thick fog is when you look in different directions.
The Angular distribution function describes the basic shape of the orbital, or the number of lobes in an orbital.
The angular distribution functions depend only on the quantum numbers $l$ and $\mathbf{m}_{\text {l }}$. That is, the angular distribution functions of all electrons with the same $l$ and $\mathbf{m}_{\mathrm{l}}$ values are the same regardless of $\mathbf{n}$ or $\mathbf{m}_{s}$. Another way of saying this is that all s orbitals have the same basic shape. For example The 2 s orbital ( $\mathrm{n}=2, l=0, \mathrm{~m}_{l}=0$ ), the $3 \mathrm{~s}(\mathrm{n}=3, l$ $\left.=0, \mathrm{~m}_{l}=0\right)$ and the $4 \mathrm{~s}\left(\mathrm{n}=, l=0, \mathrm{~m}_{l}=0\right)$ have the same basic shape (spherical)

## The radial distribution function:

The square of the radial distribution function describes the probability of finding an a electron a given distance from the nucleus.
In other words, it tells you how far a way the fog starts to tapper off, and it tell you whether or not there are pockets of clear sky in the fog.
The radial distribution function describes how far away from the nucleus the orbital extends and the number of nodes the orbital has.
The radial distribution functions depend on both $\mathbf{n}$ and $l$. This means that the number of nodes an orbital has and how far that orbital extends from the nucleus depends on the principle quantum number or energy level of the orbital (the $\mathbf{1}$ in $\mathbf{1 s}$, the $\mathbf{2}$ in $\mathbf{2 s}$, the $\mathbf{3}$ in $\mathbf{3 s}$, etc.) and the type of orbital (s vs. p vs. d).

Orbitals ( $\mathrm{n}, \mathrm{I}$, and $\mathrm{m}_{\mathrm{I}}$ )

Quantum Numbers Angular Distribution Function

$$
\begin{gathered}
1 S \\
n=1, \ell=0 \\
2 S \\
n=2, \ell=0
\end{gathered}
$$

$$
x(s)=\left(\frac{1}{4 \pi}\right)^{\frac{1}{2}}
$$

$$
x(s)=\left(\frac{1}{4 \pi}\right)^{\frac{1}{2}}
$$

$$
\chi(s)=\left(\frac{1}{4 \pi}\right)^{\frac{1}{2}}
$$

$$
\sigma=\mathrm{Zr} / \mathrm{a}_{0}
$$

$$
\begin{array}{ll}
n=2, \ell=1 & \chi\left(P_{x}\right)=\left(\frac{3}{4 \pi}\right)^{\frac{1}{2}} \sin \theta \cdot \cos \phi \\
& \chi\left(P_{y}\right)=\left(\frac{3}{4 \pi}\right)^{\frac{1}{2}} \sin \theta \cdot \sin \phi \\
& \chi\left(P_{z}\right)=\left(\frac{3}{4 \pi}\right)^{\frac{1}{2}} \cos \theta
\end{array}
$$

Radial Distribution Function

$$
\begin{aligned}
& R(1 s)=2\left(\frac{Z}{a_{0}}\right)^{\frac{3}{2}} e^{(\pi)} \\
& \text { probability of } \\
& R(2 s)=\frac{1}{2 \sqrt{2}}\left(\frac{z}{a_{0}}\right)^{\frac{3}{2}}\left(2-\frac{\sqrt{\sigma}}{0}\right) e^{\left(-\frac{\sigma}{2}\right)} \text { to } o \\
& \text { when } \sigma=2
\end{aligned}
$$

$$
\mathrm{P}(3 \mathrm{~s})=\frac{2}{81 \sqrt{3}}\left(\frac{\mathrm{z}}{\mathrm{a}_{q}}\right)^{\frac{3}{2}}\left(27-18 \sigma+2 \sigma^{2}\right) e^{\left(-\frac{\sigma}{3}\right)}
$$

two places where probabitey gales to 0

$$
R(2 p)=\frac{1}{2 \sqrt{6}}\left(\frac{Z}{a_{0}}\right)^{\frac{3}{2}} \sigma e^{\left(-\frac{\sigma}{2}\right)}
$$

change in exponent shows
$e^{-}$density falls off more slowly as are moves away from Nucleus: 3us 2

Principles of Mordern Chemistry, $\underline{2}^{\text {nd }}$ edition. Oxtoby, D.W.; Nachtrieb, N. H. Saunders College Publishing, 1990.

$$
\begin{gathered}
3 \\
l=0
\end{gathered}
$$



The Aufbau Principle

1. Start at the lowest quantum level and fill up
start at $n=1$

$$
\begin{array}{lllll}
\text { He } e_{1} & n=1 & l=0 & m_{l}=0 & m_{s}=+\frac{1}{2} \\
e_{1} & n=1 & l=0 & m_{l}=0 & m_{s}=-\frac{1}{2}
\end{array}
$$

2. Pauli exclusion principle
ran' lave identical quantum
numbers

3. Hond's Rule of Multiplicity--Multiplicity is the number of unpaired $\mathrm{e}^{-\mathrm{s}} \mathrm{s}+1$

He $H^{H}$ this is a singlet state 0 unpaired $e^{-1} s+1=1$
$\mathrm{H}+$ this is a doublet state 1 unpaired $e^{-}+1=2$
arrange $e^{-}$so that they have the highest possible multiplicity
4. Exchange Energy/Exchange Interaction

$$
11-\operatorname{cs} 1+
$$

says this is more stable doesn't matter which orbital doesn't matter which orbital 1 - - or 141 - $-~$

A quantum mechanical effect that exists between identical particles
Particles aren't actually changing positions - it is more about what happens if they were to change positions. If there would be no change, then with respect to that exchange the the change is symmetric. Symmetrical exchange for electrons spin states means that there is spacial component of the wave function is antisymmetric. There is slightly more distance between particles that have antisymmetry spacial wave functions than those with symmetric spacial wave functions. Thus, lower E.


by convention $e^{-1} s$ are placed spin up first

$\uparrow 厂$
not aligned exchange would be antisymmetric space wave function would be symmetric and the eris would experience greater $e^{-}-e^{-}$
repulsion

1. start in lowest quantum levels
2. Pauli exclusion principle
--- no two electrons in an atom or molecule can have identical quantum numbers
3. Hund's Rule of Multiplicity
--- multiplicity is the number of unpaired e-'s + 1
--- the lowest energy state for electrons in degenerate orbitals is the one with the highest multiplicity
--- electrons only pair after all degenerate orbitals have been half filled
4. Exchange interaction
--- spin aligned electrons in degenerate orbitals are lower in energy than those that aren't spin aligned

Rationalizing electron configurations/Factors affecting the energy of the electron

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Rationalizing electron configurations/Factors affecting the energy of the electron
Penetration and effective nuclear charge
$\Pi_{\mathrm{c}}=$ coulomb repulsion

- bad
- number of paired electrons
$\Pi_{\mathrm{e}}=$ exchange energy
- good in the case of parallel electrons in degenerate
orbitals in an atom
- number of exchanges that can be made and produce
identical electron configurations

Factors affecting the energy of the electron
Penetration and effective nuclear charge


Periodic Table of the Elements

|  | 1 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| (1) | 1 <br> $H$ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | 2 <br> He |
| (2) | 3 Li | 4 <br> Be |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | $\begin{aligned} & 5 \\ & \text { B } \end{aligned}$ | $\begin{aligned} & 6 \\ & \mathrm{C} \end{aligned}$ | $\begin{aligned} & 7 \\ & \mathrm{~N} \end{aligned}$ | $\begin{aligned} & 8 \\ & 0 \end{aligned}$ | $\begin{array}{\|l\|} \hline 9 \\ \mathbf{F} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 10 \\ \mathrm{Ne} \\ \hline \end{array}$ |
| (3) | $\begin{array}{\|l\|} \hline 11 \\ \mathrm{Na} \\ \hline \end{array}$ | $\begin{array}{\|c\|} \hline 12 \\ \mathbf{M g} \\ \hline \end{array}$ |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  | $\begin{array}{\|l\|l} \hline 13 \\ \text { AI } \end{array}$ | $\begin{array}{\|l\|} \hline 14 \\ \mathrm{Si} \end{array}$ | $\begin{array}{\|c\|} \hline 15 \\ \mathbf{P} \end{array}$ | $\begin{array}{\|c} \hline 16 \\ \mathrm{~S} \end{array}$ | $\begin{aligned} & 17 \\ & \mathrm{Cl} \end{aligned}$ | 18 <br> Ar |
| (4) | $\begin{aligned} & \hline 19 \\ & \mathbf{K} \end{aligned}$ | $\begin{array}{\|l\|} \hline 20 \\ \mathrm{Ca} \\ \hline \end{array}$ |  |  |  |  |  |  |  |  |  |  |  |  |  |  | $\begin{array}{\|l} \hline 21 \\ \mathrm{Sc} \\ \hline \end{array}$ | $\begin{aligned} & 22 \\ & \mathrm{Ti} \\ & \hline \end{aligned}$ | $\begin{array}{\|l\|l} 23 \\ \mathbf{V} \end{array}$ | $\begin{array}{\|l} 24 \\ \mathrm{Cr} \end{array}$ | $\begin{array}{\|l\|} \hline 25 \\ \mathrm{Mn} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 26 \\ \mathrm{Fe} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 27 \\ \mathrm{Co} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 28 \\ \mathrm{Ni} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 29 \\ \mathrm{Cu} \\ \hline \end{array}$ | $\begin{array}{\|} 30 \\ \mathbf{Z n} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 31 \\ \mathbf{G a} \\ \hline \end{array}$ | $\begin{aligned} & \hline 32 \\ & \mathbf{G e} \\ & \hline \end{aligned}$ | $\begin{array}{\|l\|} \hline 33 \\ \mathrm{As} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 34 \\ \mathrm{Se} \\ \hline \end{array}$ | $\begin{aligned} & 35 \\ & \mathrm{Br} \end{aligned}$ | 36 <br> $\mathbf{K r}$ |
| (5) | $\begin{aligned} & \hline 37 \\ & \mathbf{R b} \end{aligned}$ | $\begin{array}{\|l\|} \hline 38 \\ \mathrm{Sr} \\ \hline \end{array}$ |  |  |  |  |  |  |  |  |  |  |  |  |  |  | $\begin{array}{\|c} \hline 39 \\ \mathbf{Y} \end{array}$ | $\begin{aligned} & 40 \\ & \mathrm{Zr} \end{aligned}$ | $\begin{aligned} & 41 \\ & \mathrm{Nb} \\ & \hline \end{aligned}$ | $\begin{aligned} & \hline 42 \\ & \text { Mo } \end{aligned}$ | $\begin{aligned} & \hline 43 \\ & \text { Tc } \end{aligned}$ | $\begin{array}{\|l\|} \hline \hline \begin{array}{c} 44 \\ \mathrm{Ru} \end{array} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 45 \\ \mathbf{R h} \end{array}$ | $\begin{array}{\|l\|} \hline 46 \\ \mathrm{Pd} \end{array}$ | $\begin{aligned} & \hline 47 \\ & \mathrm{Ag} \end{aligned}$ | $\begin{aligned} & \hline 48 \\ & \mathrm{Cd} \end{aligned}$ | $\begin{array}{\|l\|} \hline 49 \\ \text { In } \end{array}$ | $\begin{array}{\|l\|} \hline 50 \\ \mathbf{S n} \end{array}$ | $\begin{array}{\|l\|} \hline 51 \\ \mathrm{Sb} \end{array}$ | $\begin{aligned} & \hline 52 \\ & \mathrm{Te} \end{aligned}$ | $\begin{gathered} 53 \\ 1 \end{gathered}$ | $\begin{array}{\|l\|} \hline 54 \\ \mathrm{Xe} \end{array}$ |
| (6) | $\begin{array}{\|l\|} \hline 55 \\ \mathrm{Cs} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 56 \\ \mathrm{Ba} \\ \hline \end{array}$ | $\begin{aligned} & 57 \\ & \text { La } \end{aligned}$ | $\begin{aligned} & 58 \\ & \mathrm{Ce} \\ & \hline \hline \end{aligned}$ | $\begin{aligned} & 59 \\ & \mathrm{Pr} \end{aligned}$ | $\begin{aligned} & \hline 60 \\ & \mathrm{Nd} \end{aligned}$ | $\begin{array}{\|l\|} \hline 61 \\ \mathrm{Pm} \\ \hline \end{array}$ | $\begin{array}{c\|} \hline 62 \\ \mathrm{Sm} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 63 \\ \mathrm{Eu} \\ \hline \end{array}$ | $\begin{aligned} & 64 \\ & \mathbf{G d} \end{aligned}$ | $\begin{aligned} & 65 \\ & \mathrm{~Tb} \\ & \hline \end{aligned}$ | $\begin{aligned} & \hline 66 \\ & \text { Dy } \end{aligned}$ | $\begin{array}{\|l\|} \hline 67 \\ \mathrm{Ho} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 68 \\ \mathrm{Er} \end{array}$ | $\begin{array}{\|l\|} \hline 69 \\ \mathrm{Tm} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 70 \\ \mathrm{Yb} \end{array}$ | $\begin{array}{\|l\|} \hline 71 \\ \mathrm{Lu} \end{array}$ | $\begin{aligned} & \hline 72 \\ & \mathrm{Hf} \end{aligned}$ | $\begin{aligned} & \hline 73 \\ & \mathrm{Ta} \end{aligned}$ | $\begin{aligned} & \hline 74 \\ & \mathbf{W} \\ & \hline \end{aligned}$ | $\begin{array}{\|l\|} \hline 75 \\ \mathrm{Re} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 76 \\ \text { Os } \\ \hline \end{array}$ | $\begin{aligned} & \hline 77 \\ & \mathbf{I r} \end{aligned}$ | $\begin{array}{\|l} \hline 78 \\ \mathrm{Pt} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 79 \\ \mathbf{A u} \end{array}$ | $\begin{aligned} & \hline 80 \\ & \mathrm{Hg} \\ & \hline \end{aligned}$ | $\begin{array}{\|l\|} \hline 81 \\ \mathrm{TI} \\ \hline \end{array}$ | $\begin{array}{\|l\|} \hline 82 \\ \mathrm{~Pb} \\ \hline \end{array}$ | $\begin{aligned} & \hline 83 \\ & \mathrm{Bi} \end{aligned}$ | $\begin{array}{\|l\|} \hline 84 \\ \mathrm{Po} \\ \hline \end{array}$ | $\begin{aligned} & \hline 85 \\ & \text { At } \end{aligned}$ | $\begin{array}{\|l\|} \hline 86 \\ \text { Rn } \\ \hline \end{array}$ |
| (7) | $\begin{aligned} & \hline 87 \\ & \mathrm{Fr} \end{aligned}$ | $\begin{array}{\|l\|} \hline 88 \\ \text { Ra } \end{array}$ | $\begin{aligned} & 89 \\ & \mathbf{A c} \end{aligned}$ | $\begin{aligned} & \hline 90 \\ & \mathrm{Th} \end{aligned}$ | $\begin{aligned} & \hline 91 \\ & \mathrm{~Pa} \end{aligned}$ | $\begin{aligned} & 92 \\ & \mathbf{U} \end{aligned}$ | $\begin{array}{\|l\|} \hline 93 \\ \mathrm{~Np} \end{array}$ | $\begin{aligned} & 94 \\ & \mathrm{Pu} \end{aligned}$ | $\begin{array}{\|c\|} \hline 95 \\ \text { Am } \end{array}$ | $\begin{aligned} & \hline 96 \\ & \mathrm{Cm} \end{aligned}$ | $\begin{aligned} & \hline 97 \\ & \text { Bk } \end{aligned}$ | $\begin{aligned} & 98 \\ & \mathrm{Cf} \end{aligned}$ | $\begin{array}{\|c\|} \hline 99 \\ \text { Es } \end{array}$ | $\begin{array}{\|l\|} \hline 100 \\ \mathrm{Fm} \end{array}$ | $\begin{array}{\|l\|} \hline 101 \\ \mathrm{Md} \end{array}$ | $\begin{aligned} & 102 \\ & \text { No } \end{aligned}$ | $\begin{gathered} 103 \\ \mathbf{L r} \end{gathered}$ | $\\| \begin{aligned} & 104 \\ & \mathbf{R f} \end{aligned}$ | Db | $\begin{aligned} & 106 \\ & \mathrm{Sg} \end{aligned}$ | $\begin{aligned} & 107 \\ & \text { Bh } \end{aligned}$ | $\begin{aligned} & \hline 108 \\ & \mathrm{Hs} \end{aligned}$ | $\begin{aligned} & 109 \\ & \mathbf{M t} \end{aligned}$ | $\begin{array}{\|l\|} \hline 110 \\ \mathrm{Ds} \end{array}$ | $\begin{array}{\|l\|} \hline 111 \\ \mathrm{Rg} \\ \hline \end{array}$ | $\begin{aligned} & 112 \\ & \mathbf{C n} \end{aligned}$ | $\begin{aligned} & \hline 113 \\ & \mathrm{Nh} \end{aligned}$ | $\begin{gathered} \\ \hline 114 \\ \mathrm{FI} \end{gathered}$ | $\begin{aligned} & \hline 115 \\ & \mathrm{Mc} \end{aligned}$ | $\begin{array}{\|c} 116 \\ \mathrm{Lv} \end{array}$ | $\begin{gathered} 117 \\ \mathrm{Ts} \end{gathered}$ | $\begin{aligned} & 118 \\ & \mathbf{O g} \end{aligned}$ |

## Wave Functions

http://www.westfield.ma.edu/cmasi/advinorg/angular_distribution_functions/text_and_graphics_containe.htm

