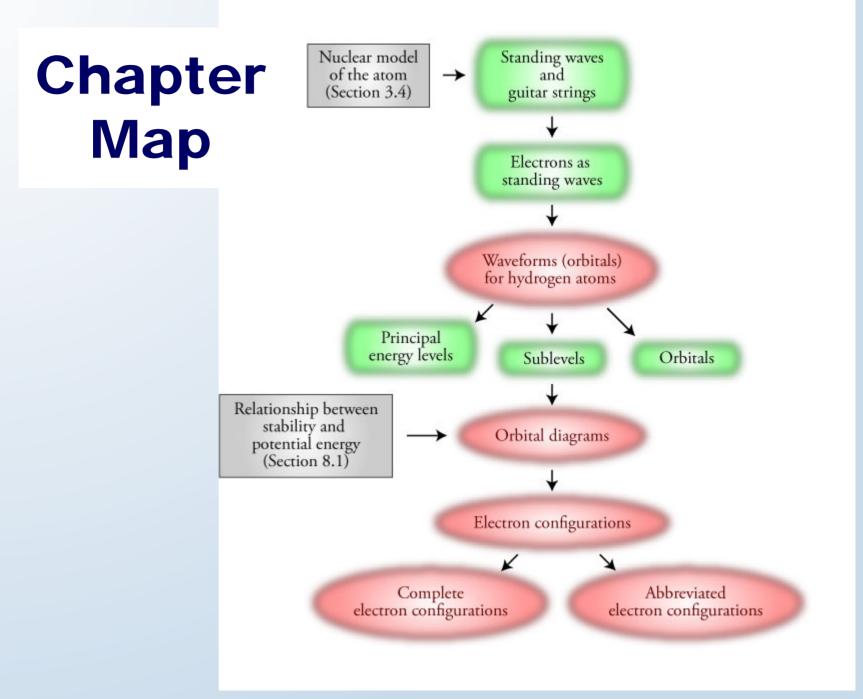
#### **Chapter 11**

#### **Modern Atomic Theory**





# **Atomic Theory**

- To see a World in a Grain of Sand And a Heaven in a Wild Flower Hold Infinity in the palm of your hand And Eternity in an hour William Blake Auguries of Innocence
- Thus, the task is not so much to see what no one has yet seen, but to think what nobody has yet thought, about that which everybody sees.
  Erwin Schrodinger

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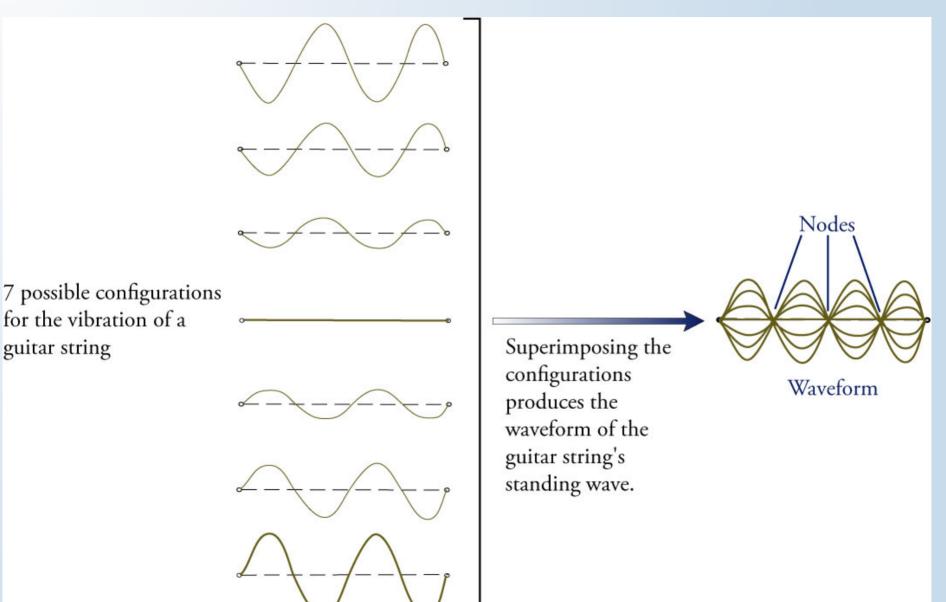
#### Ways to deal with Complexity and Uncertainty

- Analogies In order to communicate something of the nature of the electron, scientists often use analogies. For example, in some ways, electrons are *like* vibrating guitar strings.
- Probabilities In order to accommodate the uncertainty of the electron's position and motion, we refer to where the electron *probably is* within the atom instead of where it definitely is.

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#### **Guitar String Waveform**

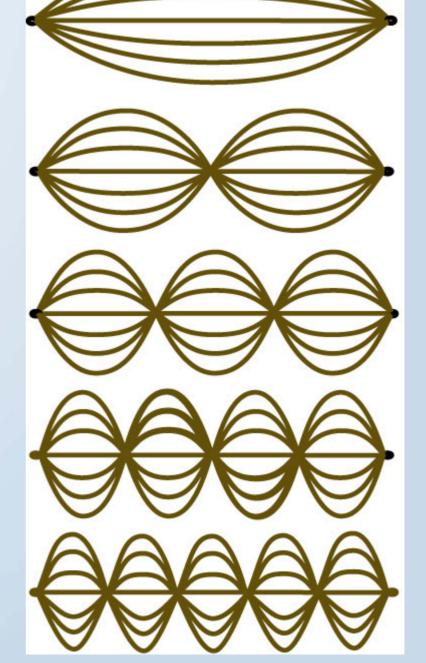


Allowed Vibrations for a Guitar String

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# Wave Character of the Electron

- Just as the intensity of the movement of a guitar string can vary, so can the intensity of the negative charge of the electron vary at different positions outside the nucleus.
- The variation in the intensity of the electron charge can be described in terms of a three-dimensional standing wave *like* the standing wave of the guitar string.

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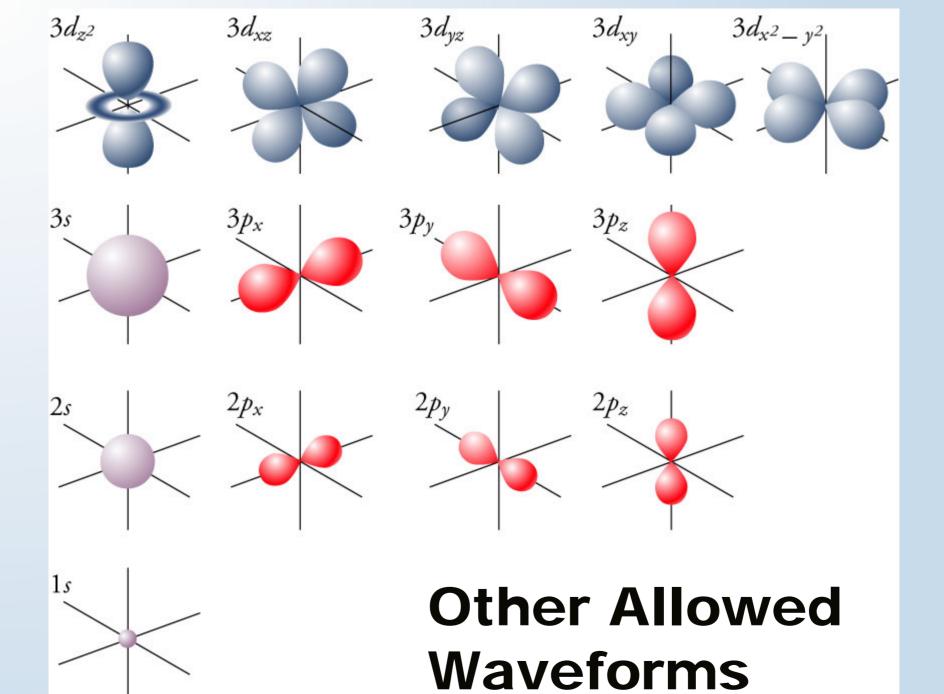
# Wave Character of the Electron

- Although both the electron and the guitar string can have an infinite number of possible waveforms, only certain waveforms are possible.
- We can focus our attention on the waveform of varying charge intensity without having to think about the actual physical nature of the electron.

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#### Waveform for 1*s* Electron (with quantum numbers 1,0,0)

Nucleus, about 0.000001 ~ the diameter of the atom  The negative charge is most intense at the nucleus and decreases in intensity with distance outward.



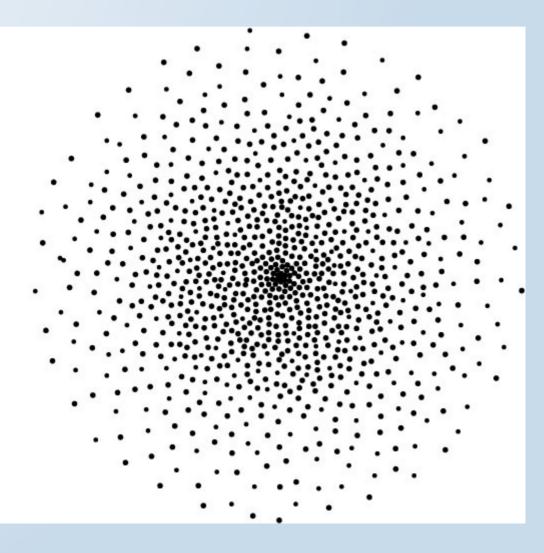
# 1s Orbital

Almost all of the electron's charge lies within a spherical shell with the diameter of this circle.

Sphere enclosing almost all of the electron's negative charge

# Particle Interpretation of 1s Orbital

A multiple exposure picture of the electron in a 1*s* orbital of a hydrogen atom might look like this.



### 2s Orbital

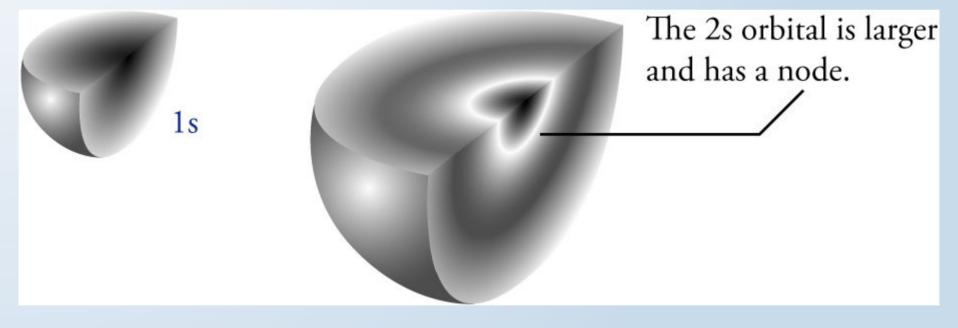
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 The 2s orbital for a hydrogen atom is larger than the 1s orbital and has a node, which is a region within the orbital where the charge intensity decreases to zero.

# Cutaway of 1s and 2s Orbitals (with quantum numbers 2,0,0)



#### Ground State and Excited State

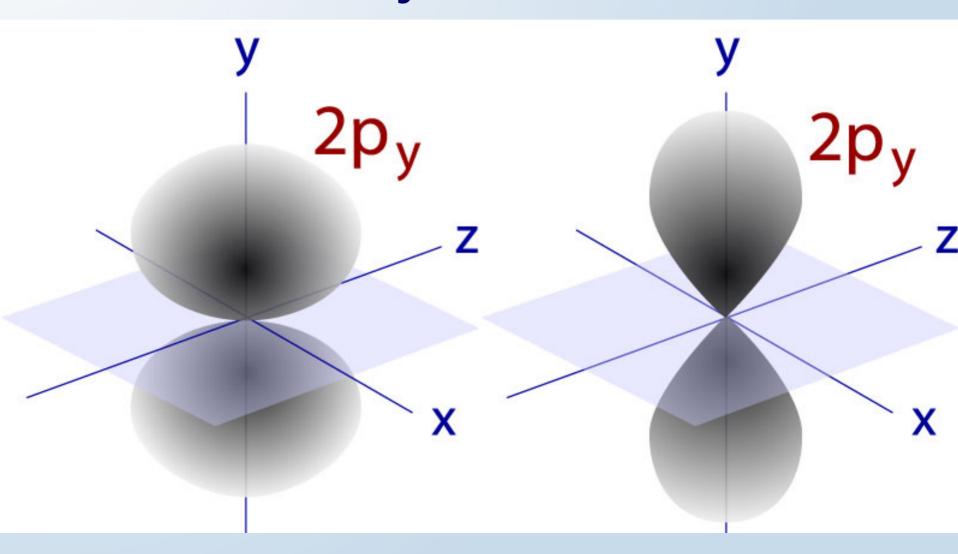
- Hydrogen atoms with their electron in the 1s orbital are said to be in their ground state.
- A hydrogen atom with its electron in the 2s orbital is in an *excited* state.

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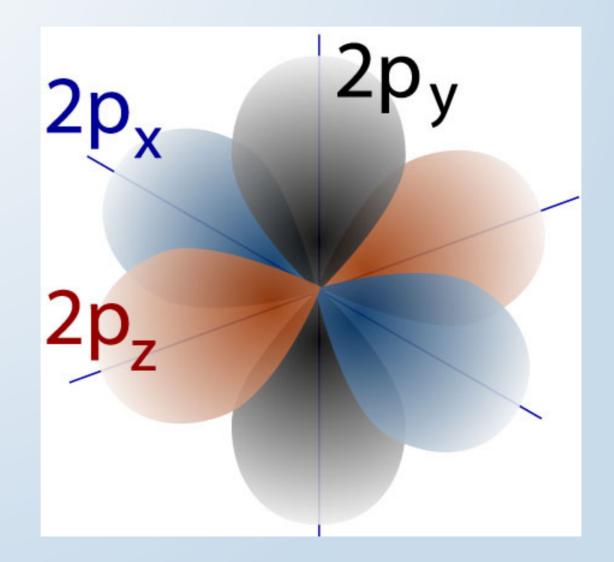
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### Realistic and Stylized 2p<sub>y</sub> Orbital



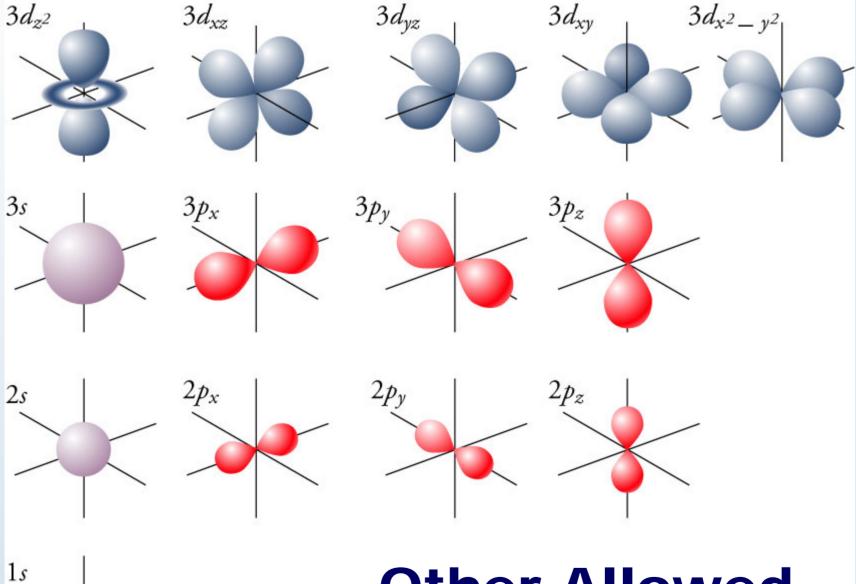
# $2p_{x}$ , $2p_{y}$ , and $2p_{z}$ Orbitals

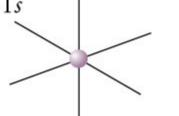


#### 3d Orbitals

Four of the five 3*d* orbitals have a double dumbbell shape like this one.

The fifth 3*d* orbital is shaped like a dumbell and a donut.





#### Other Allowed Waveforms

#### **Sublevels**

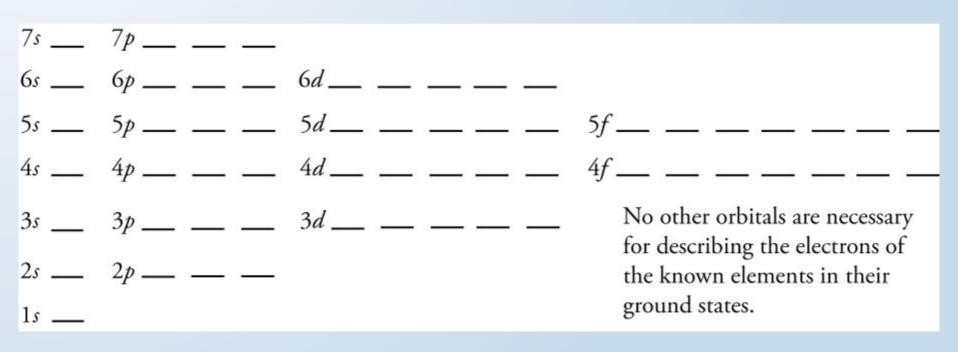
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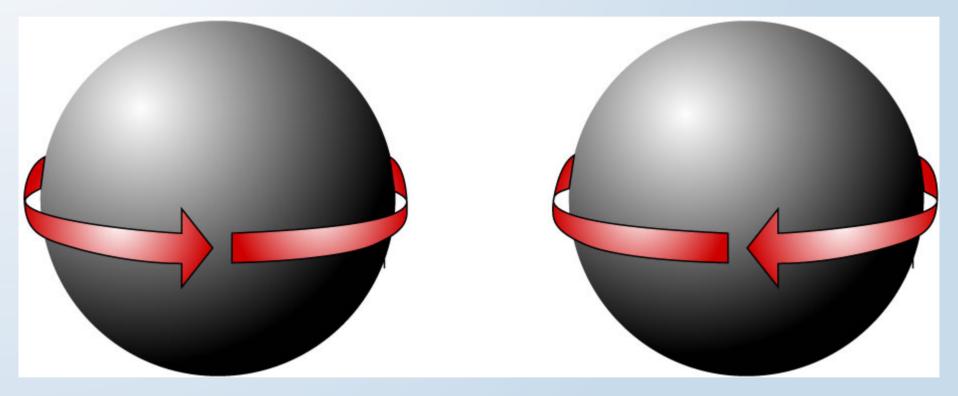
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- Orbitals that have the same potential energy, the same size, and the same shape are in the same *sublevel*.
- The sublevels are sometimes called *subshells*.

### Orbitals for Ground States of Known Elements



#### **Electron Spin**



#### **Pauli Exclusion Principle**

- No two electrons in an atom can be the same in all ways.
- There are four ways that electrons can be the same:
  - Electrons can be in the same principal energy level.
  - They can be in the same sublevel.
  - They can be in the same orbital.
  - They can have the same spin.

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# Ways to Describe Electrons in Atoms

 Arrows are added to an orbital diagram to show the distribution of electrons in the possible orbitals and the relative spin of each electron. The following is an orbital diagram for a nitrogen atom.

$$2s \stackrel{\uparrow\downarrow}{1s} 2p \stackrel{\uparrow}{1s} \frac{\uparrow\downarrow}{1s}$$

• The information in orbital diagrams is often described in a shorthand notation called an *electron configuration*.

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$$1s^2 2s^2 2p^3$$

#### **Electron Configurations**

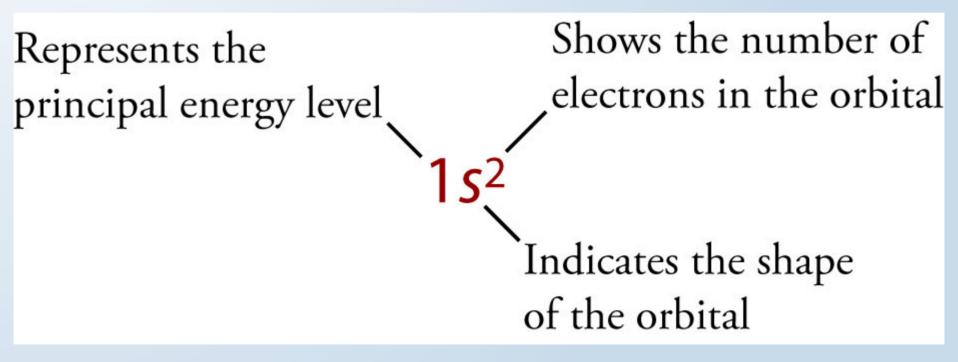
- The sublevels are filled in such a way as to yield the lowest overall potential energy for the atom.
- No two electrons in an atom can be the same in all ways. This is one statement of the *Pauli Exclusion Principle*.
- When electrons are filling orbitals of the same energy, they prefer to enter empty orbitals first, and all electrons in half-filled orbitals have the same spin. This is called *Hund's Rule*.

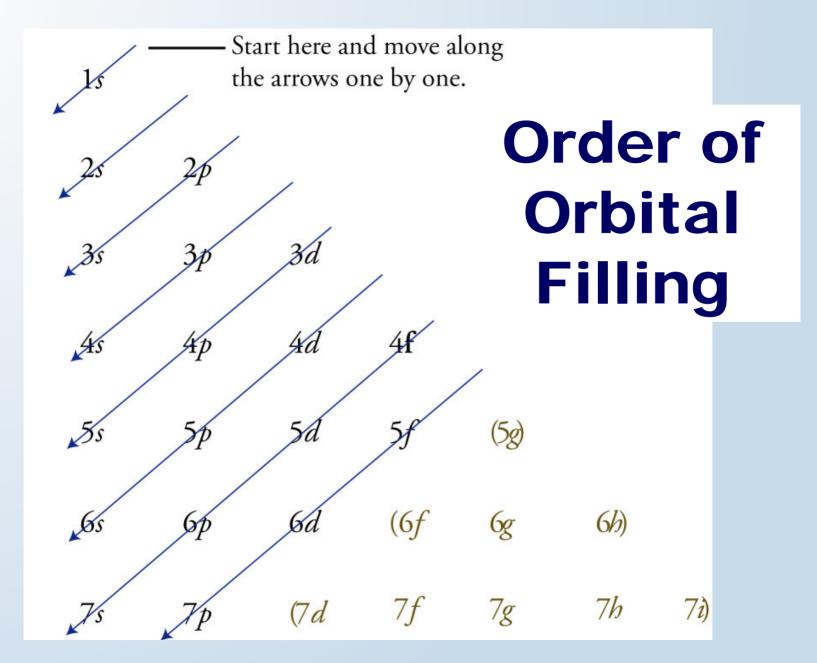
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# Electron Configurations (cont.)





1s 2s 2p 3s 3p 4s 3d 4p 5s 4d 5p 6s 4f 5d 6p 7s 5f 6d 7p

#### Writing Electron Configurations

- Determine the number of electrons in the atom from its atomic number.
- Add electrons to the sublevels in the correct order of filling.
- Add two electrons to each s sublevel, 6 to each p sublevel, 10 to each d sublevel, and 14 to each f sublevel.
- To check your complete electron configuration, look to see whether the location of the last electron added corresponds to the element's position on the periodic table.

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# Order of Filling from the Periodic Table

																				18
	s bl	ock									_		o bla	ock 8A						
	1	2									12	1			13	14	15	16	17	2
	1A	2A									ls				3A	4A	5A	6A	7A	
2 <i>s</i>	3	4						d b	lock		_			2p	5	6	7	8	9	10
	11	12		3	4	5	6	7	8	9	10	11	12		13	14	15	16	17	18
35				3B	4B	5B	6B	7B	<b>8</b> B	8B	<b>8</b> B	1B	2B	3p						
4 <i>s</i>	19	20	3 <i>d</i>	21	22	23	24	25	26	27	28	29	30	4 <i>p</i>	31	32	33	34	35	36
55	37	38	4 <i>d</i>	39	40	41	42	43	44	45	46	47	48	5p	49	50	51	52	53	54
<u>6</u> s	55	56	5d	71	72	73	74	75	76	77	78	79	80	6p	81	82	83	84	85	86
7 <i>s</i>	87	88	6d	103	104	105	106	107	108	109	110	111	112	7p	113	114	115	116	117	118

#### fblock

4 <i>f</i>	57	58	59	60	61	62	63	64	65	66	67	68	69	70
5f	89	90	91	92	93	94	95	96	97	98	99	100	101	102

# Long Periodic Table

s bl	block																							p block				18 8A			
1 1A	2 2A	2																						1 1s		13 3A	14 4A	15 5A	16 6A	17 7A	2
3 25	4														d block $\frac{5}{2p}$ 6										6	7	8	9	10		
11 3s	12	1														3 3B	4 4B	5 5B	6 6B	7 7B	8 8B	9 8B	10 8B	11 1B	12 2B	13 3p	14	-15	16	17	18
19 4s	20	20														21 3d	22	23	24	25	26	27	28	29	30	31 4p	32	33	34	35	36
37 5s	<sup>38</sup> <i>f</i> block													39 4d	40	41	42	43	44	45	46	47	48	49 5p	50	-51	52	53	54		
55 6s	56	57 4f	58	59	60	61	62	63	64	65	66	67	68	69	70	71 5d	72	73	74	75	76	77	78	79	80	81 6p	82	83	84	85	86
87 7s	88	89 5f	90	91	92	93	94	95	96	97	98	99	100	101	102	103 6d	104	105	106	107	108	109	110	111	112	113 7p	114	115	116	117	118

#### Drawing Orbital Diagrams

- Draw a line for each orbital of each sublevel mentioned in the complete electron configuration. Draw one line for each s sublevel, three lines for each p sublevel, five lines for each d sublevel, and seven lines for each f sublevel.
- Label each sublevel.

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- For orbitals containing two electrons, draw one arrow up and one arrow down to indicate the electrons' opposite spin.
- For unfilled sublevels, follow Hund's Rule.

### Abbreviated Electron Configurations

- The highest energy electron are most important for chemical bonding.
- The noble gas configurations of electrons are especially stable and, therefore, not important for chemical bonding.
- We often describe electron configurations to reflect this representing the noble gas electrons with a noble gas symbol in brackets.
- For example, for sodium

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 $1s^2 2s^2 2p^6 3s^1$  goes to [Ne]  $3s^1$ 

#### Writing Abbreviated Electron Configurations

- Find the symbol for the element on a periodic table.
- Write the symbol in brackets for the noble gas located at the far right of the preceding horizontal row on the table.
- Move back down a row (to the row containing the element you wish to describe) and to the far left. Following the elements in the row from left to right, write the outer-electron configuration associated with each column until you reach the element you are describing.

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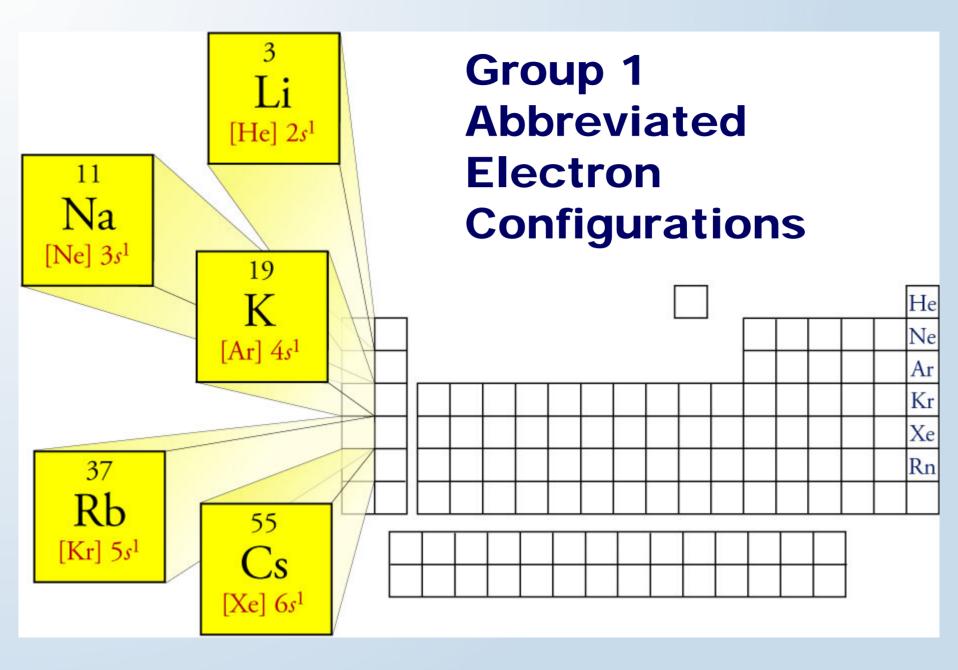
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Abbreviated Electron Configurations – Optional Step

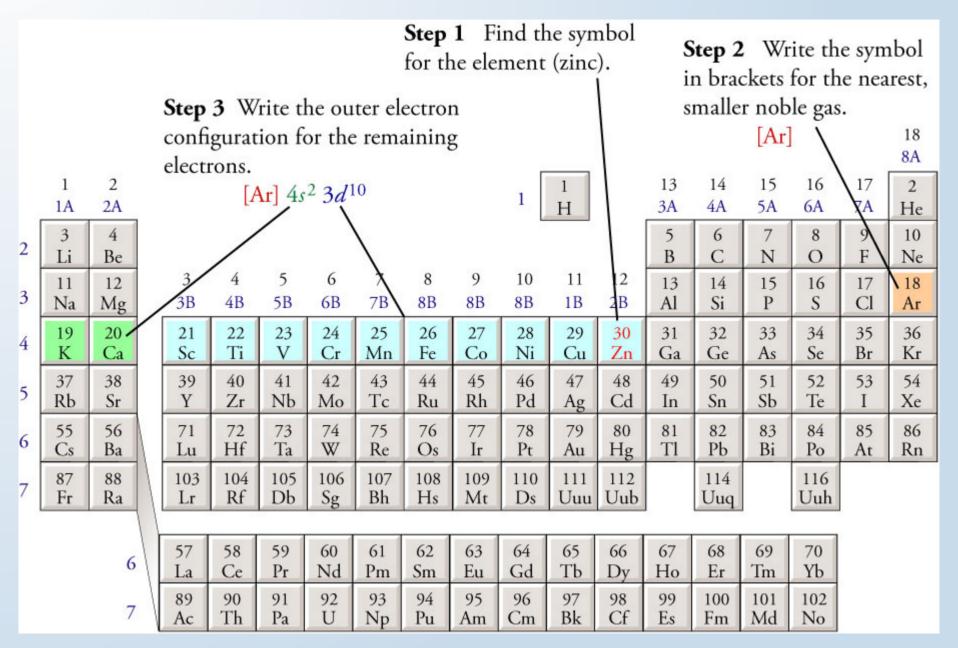
 Rewrite the abbreviated electron configuration, listing the sublevels in the order of increasing principal energy level (all of the 3's before the 4's, all of the 4's before the 5's, etc.)

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#### **Abbreviated Electron Configuration Steps for Zinc**



#### **Common Mistakes**

- Complete electron configurations miscounting electrons (Use the periodic table to determine order of filling.)
- Orbital diagrams forgetting to leave electrons unpaired with the same spin when adding electrons to the *p*, *d*, or *f* sublevels (Hund's Rule)
- Abbreviated electron configurations
  - Forgetting to put 4f<sup>14</sup> after [Xe]

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- Forgetting to list sublevels in the order of increasing principal quantum number
- For cations, forgetting to remove highest energy level electrons first