

The Quantum-Mechanical Model of the Atom

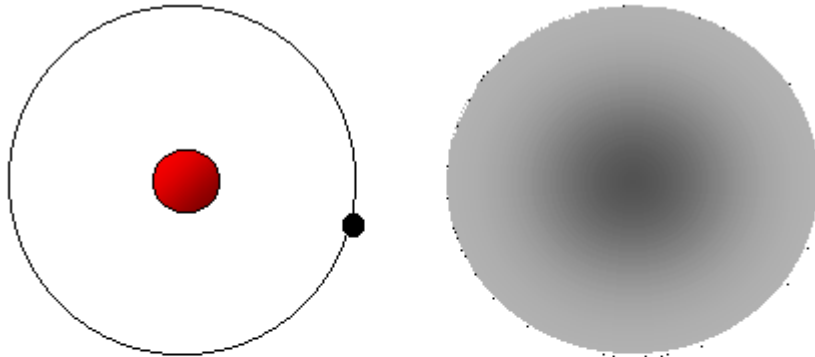


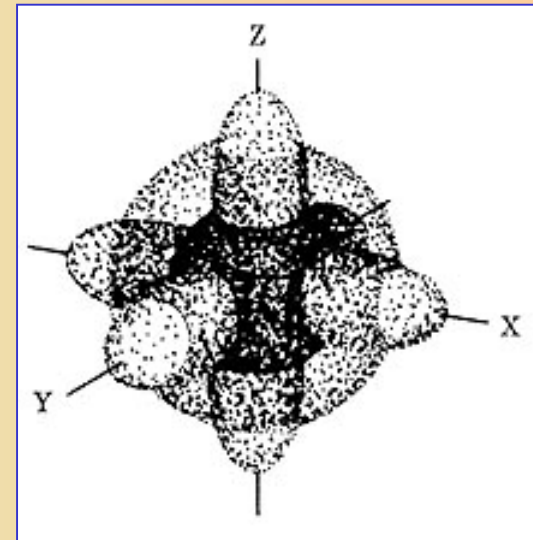
Figure 8: Two views of the hydrogen atom. The model at right views the electron as a "probability cloud."

<http://pages.prodigy.net/sullydog/archives/qm/image20.gif>

Introduction

Acceptance of the dual nature of matter and energy and of the uncertainty principle culminated with the quantum-mechanical model of the hydrogen atom.

<http://www.kennethsnelson.net/atom/2-SchrodAtm.jpg>



The Quantum-Mechanical Model of the Atom

The atomic orbital and the probable location of the electron

The Bohr's orbit was a path followed by the electron; the **orbital** is a mathematical function that can show the probability to find the electron in a given spatial region.

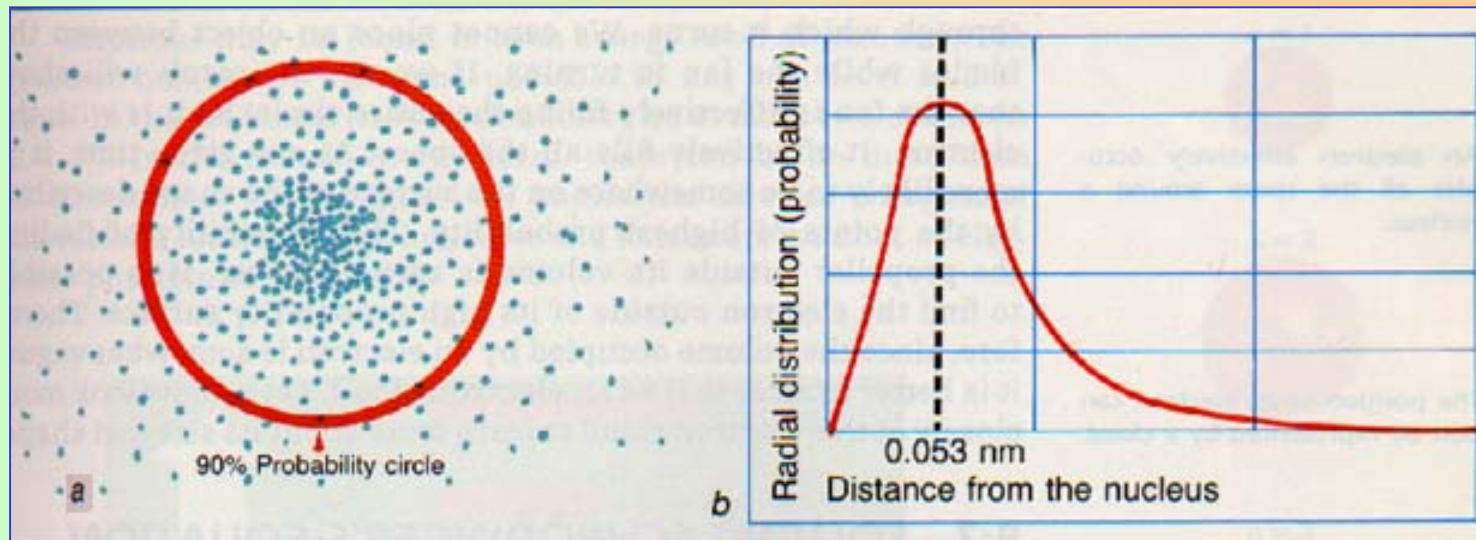


FIGURE 9-4. Probability plots for a hydrogen electron are shown in (a). Note the area represented by 90% probability. The point of highest probability for a hydrogen electron occurs at about 0.053 nm from the nucleus (b).

<http://boomeria.org/chemtextbook/fig9-4.jpg>

The Quantum-Mechanical Model of the Atom

Relationship Among Values of n , l , and m_l Through $n = 4$

n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1s	0	1	1
2	0	2s	0	1	4
	1	2p	1, 0, -1	3	
3	0	3s	0	1	9
	1	3p	1, 0, -1	3	
	2	3d	2, 1, 0, -1, -2	5	
4	0	4s	0	1	16
	1	4p	1, 0, -1	3	
	2	4d	2, 1, 0, -1, -2	5	
	3	4f	3, 2, 1, 0, -1, -2, -3	7	

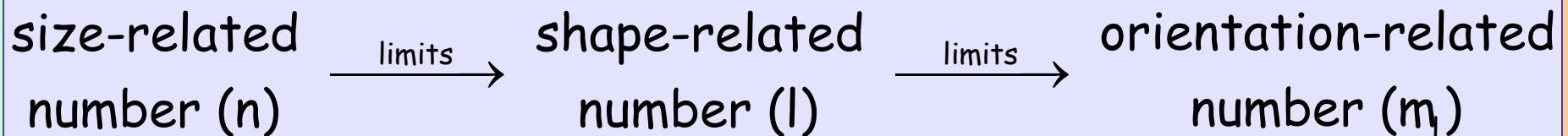
http://www.chem.ufl.edu/~itl/2045_s99/matter/TB06_002.GIF

Quantum numbers of an atomic orbital

An atomic orbital is specified by three quantum numbers:

- one is related to the orbital's **size**
- another to its **shape**, and
- the third to its **orientation** in space.

The quantum numbers have a hierarchical relationship:



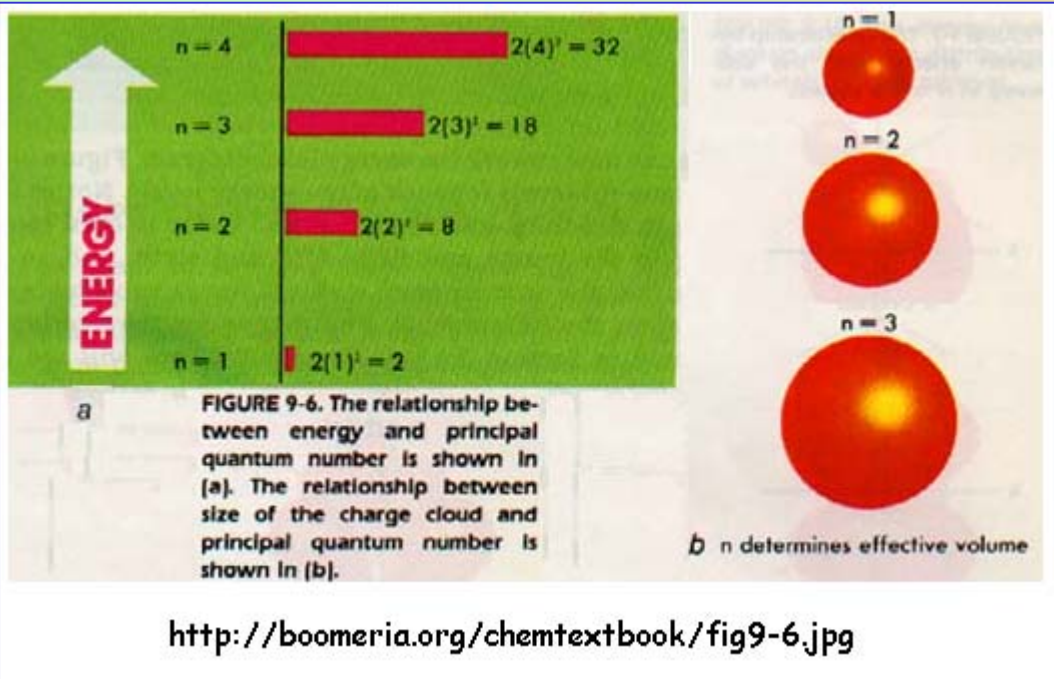
The Quantum-Mechanical Model of the Atom

Quantum numbers of an atomic orbital

The principal quantum number (n) is a positive integer (1, 2, 3...).

It indicates the relative size of the orbital and therefore the relative distance from the nucleus.

The higher the n value, the higher the energy level.



size-related

number (n)

1, 2, 3, ...

limits →

shape-related

number (l)

0 to $n-1$

limits →

orientation-related

number (m_l)

-1, ..., 0, ... +1

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http://www.chem.ufl.edu/~itl/2045_s99/matter/TB06_002.6IF

The angular momentum quantum number (l) is an integer from 0 to $n-1$. It is related to the shape of the orbital and is sometimes called the orbital-shape quantum number.

The principal quantum number sets a limit on its values. For orbitals with $n=2$, l can have a value of 0 or 1; for those with $n=3$, l can be 0, 1, or 2.

size-related

number (n)

1, 2, 3, ...

limits →

shape-related

number (l)

0 to $n-1$

limits →

orientation-related

number (m_l)

-1, ..., 0, ... +1

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	3	4f	3, 2, 1, 0, -1, -2, -3	7	

http://www.chem.ufl.edu/~itl/2045_s99/matter/TB06_002.GIF

Quantum numbers of an atomic orbital

The magnetic quantum number (m_l) is an integer from $-l$ through 0 to $+l$.

It prescribes the orientation of the orbital in the space around the nucleus.

size-related

number (n)

1, 2, 3, ...

limits →

shape-related

number (l)

0 to $n-1$

limits →

orientation-related

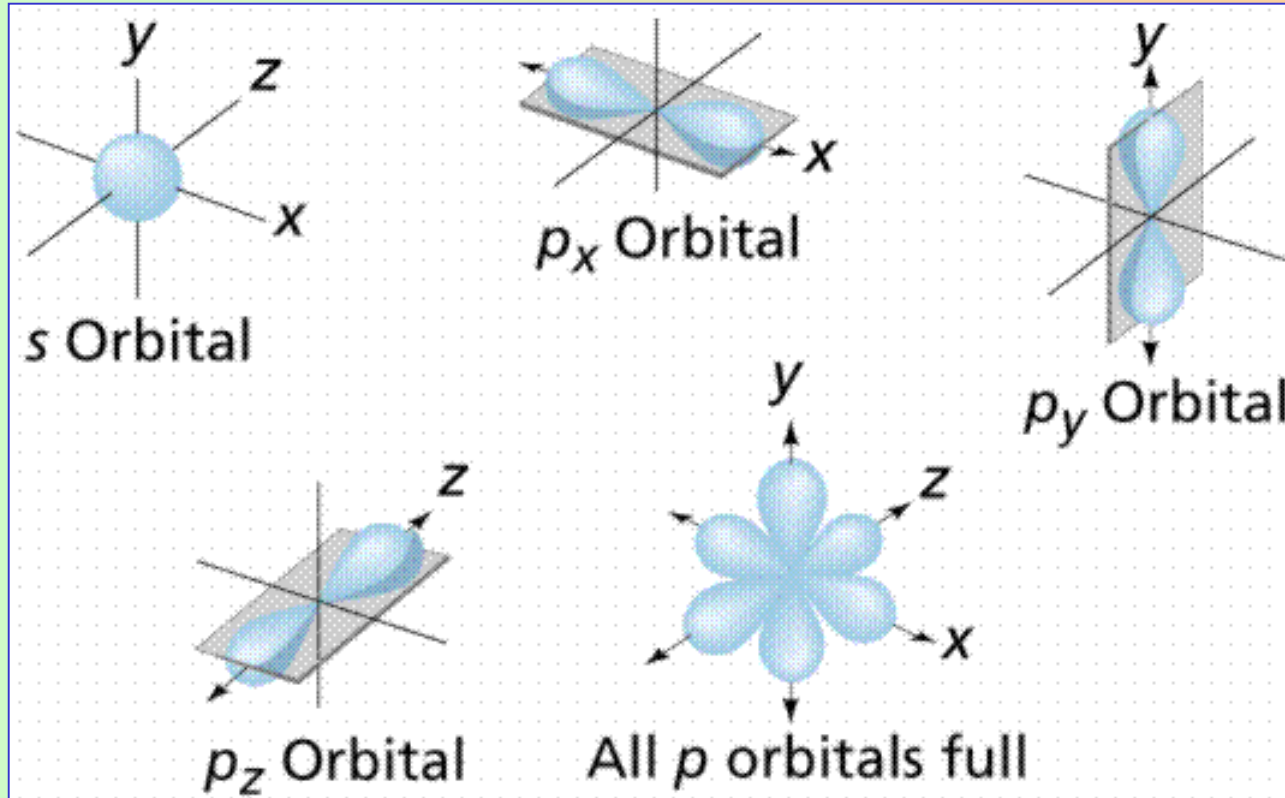
number (m_l)

$-l, \dots, 0, \dots, +l$

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Shapes of atomic orbitals

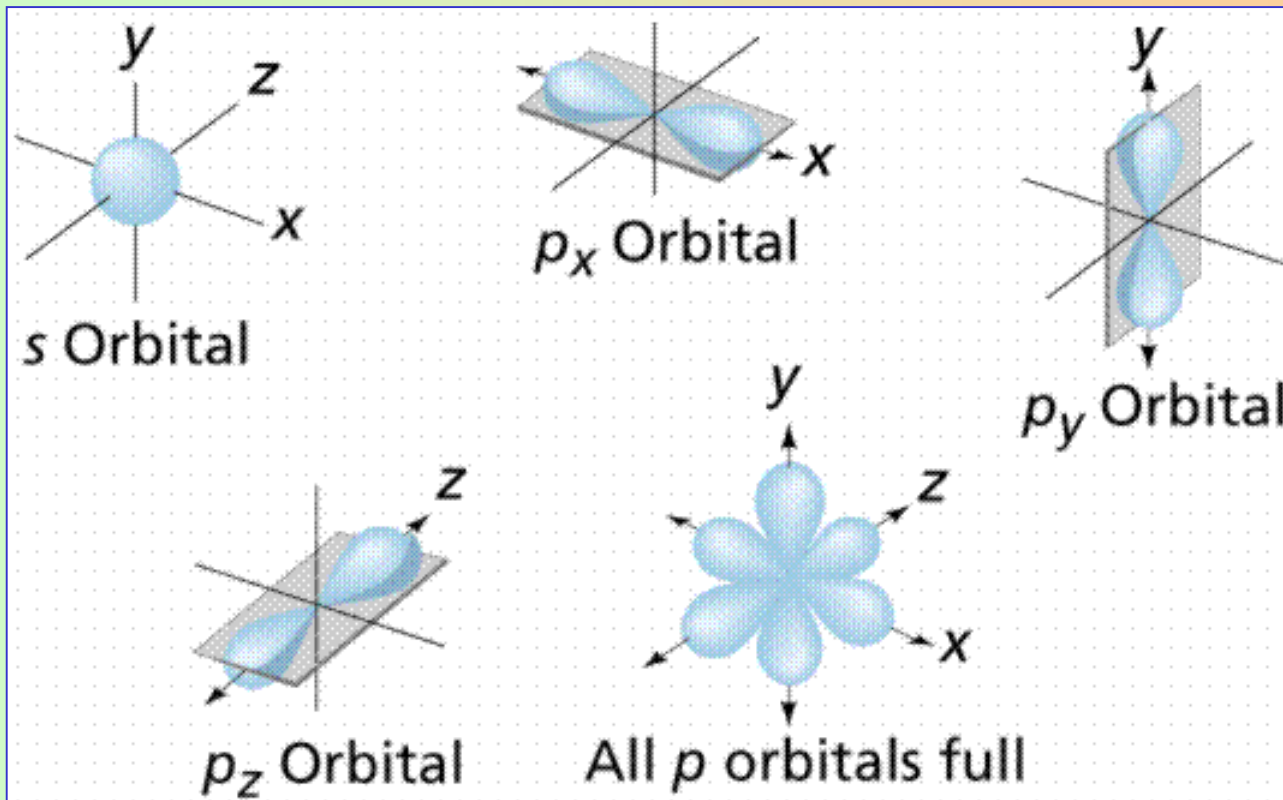
The “s” orbital: an orbital with $l=0$ has a **spherical** shape with the nucleus at its center and is called an s orbital.



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Shapes of atomic orbitals

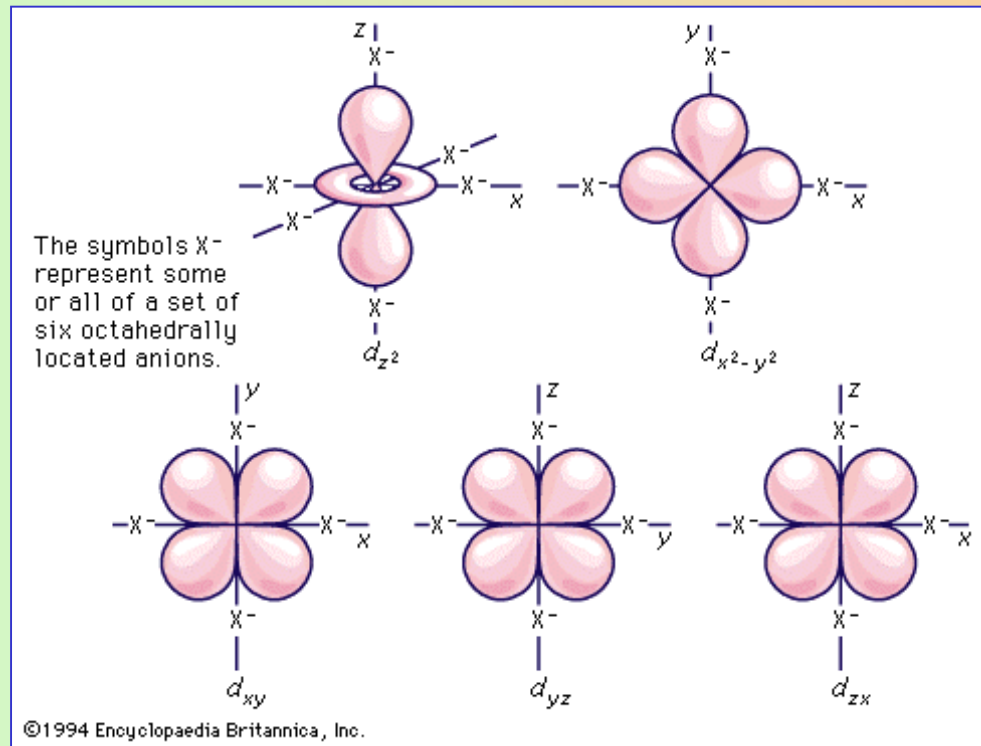
The “p” orbital: an orbital with $l=1$ has two regions (lobes) of high probability, one either side of the nucleus and is called a p orbital. Each p orbital has a specific orientation in space.



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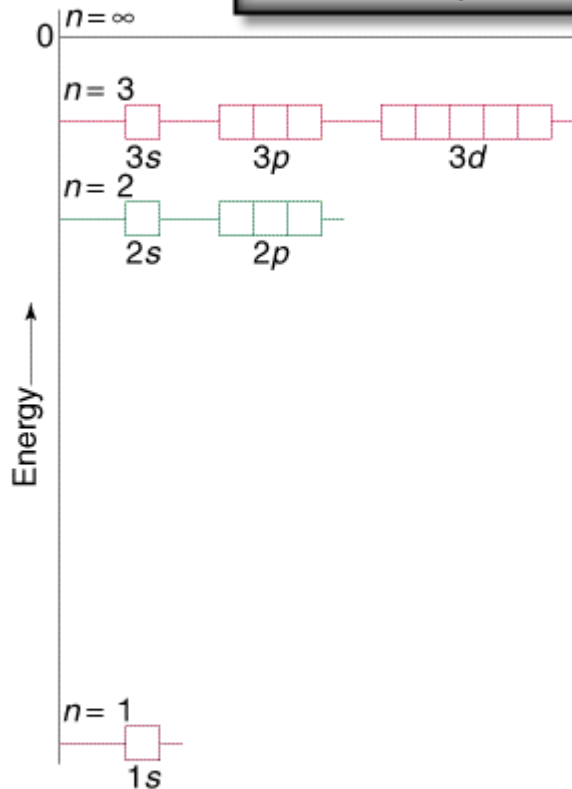
Shapes of atomic orbitals

The “d” orbital: an orbital with $l=2$ is called a d orbital. There are five possible m_l values for the $l=2$ value: $-2, -1, 0, +1,$ and $+2$. This, a d orbital can have any one of five different orientations.



The Quantum-Mechanical Model of the Atom

Hydrogen atom: energy levels



http://www.chem.ufl.edu/~itl/2045_s99/matter/FG06_019.GIF

Energy levels of the hydrogen atom

The energy state of the H atom depends on the principal quantum number n only.

An electron in an orbital with higher n value spends its time, on the average, farther from the nucleus, so it is higher in energy.