Quantum Numbers, Orbitals, and Probability Patterns

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Concept 1 Quantum Numbers, Orbitals, and Probability Patterns

Lesson Objectives

The student will:

- state the relationship between the principal quantum number (n), the number of orbitals, and the maximum number of electrons in a principal energy level.

Vocabulary

- Pauli exclusion principle
- principal quantum number
- quantum number

Introduction

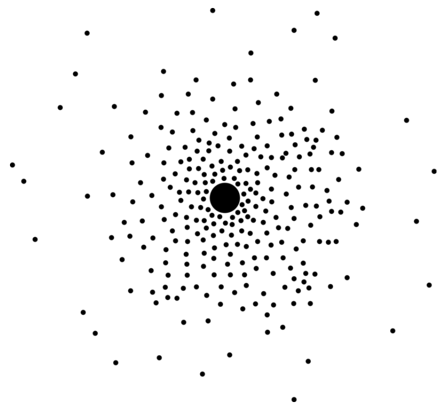
Erwin Schrödinger proposed a wave equation for electron matter waves that was similar to the known equations for other wave motions in nature. This equation describes how a wave associated with an electron varies in space as the electron moves under various forces. Schrödinger worked out the solutions of his equation for the hydrogen atom, and the results agreed perfectly with the known energy levels for hydrogen. Furthermore, the equation could be applied to more complicated atoms. It was found that Schrodinger's equation gave a correct description of an electron's behavior in almost every case. In spite of the overwhelming success of the wave equation in describing electron energies, the very meaning of the waves was vague and unclear.

There are very few scientists who can visualize the behavior of an electron as a standing wave during chemical bonding or chemical reactions. When chemists are asked to describe the behavior of an electron in an electrochemical cell, they do not use the mathematical equations of quantum mechanics, nor do they discuss standing waves. The behavior of electrons in chemical reactions is best understood by considering the electrons to be particles.

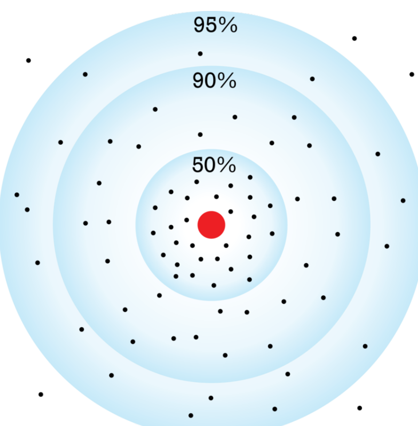
A physicist named Max Born was able to attach some physical significance to the mathematics of quantum mechanics. Born used data from Schrodinger's equation to show the probability of finding the electron (as a particle) at the point in space for which the equation was solved. Born's ideas allowed chemists to visualize the results of Schrodinger's wave equation as probability patterns for electron positions.

Probability Patterns

Suppose we had a camera with such a fast shutter speed that it could capture the position of an electron at any given moment. We could take a thousand pictures of this electron at different times and find it at many different positions in the atom. We could then plot all the electron positions onto one picture, as seen in the sketch below.

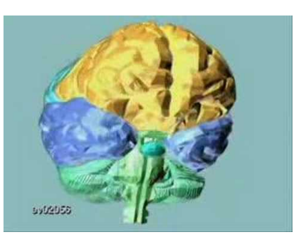


One way of looking at this picture is as an indication of the probability of where you are likely to find the electron in this atom. Keep in mind that this image represents an atom with a single electron. The dots do not represent different electrons; the dots are positions where the single electron can be found at different times. From this image, it is clear that the electron spends more time near the nucleus than it does far away. As you move away from the nucleus, the probability of finding the electron becomes less and less. It is important to note that there is no boundary in this picture. In other words, there is no distance from the nucleus where the probability of finding an electron becomes zero. However, for much of the work we will be doing with atoms, it is convenient (even necessary) to have a boundary for the atom. Most often, chemists arbitrarily draw in a boundary for the atom, choosing some distance from the nucleus beyond which the probability of finding the electron becomes very low. Frequently, the boundary is placed such that 90% of the probability of finding the electron is inside the boundary.



The image above shows boundaries drawn in at 50%, 90%, and 95% probability of finding the electron within the boundary. It is important to remember that the boundary is there for our convenience, and there is no actual boundary on an atom. This probability plot is very simple because it is for the first electron in an atom. As the atoms become more complicated (more energy levels and more electrons), the probability plots also become more complicated.

All of the scientists whose names appear in the "Atom Song" have appeared in our book. Please watch the video: http://www.youtube.com/watch?v=vUzTQWn-wfE (3:28).



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The Principal Quantum Number

Solutions to Schrödinger's equation involve four special numbers called **quantum numbers**. (Three of the numbers come from Schrödinger's equation, and the fourth one comes from an extension of the theory.) These four numbers completely describe the energy of an electron. Each electron has exactly four quantum numbers, and no two electrons have the same four numbers. The statement that no two electrons can have the same four quantum numbers is known as the **Pauli exclusion principle**.

The **principal quantum number** is a positive integer (1, 2, 3, . . . *n*) that indicates the main energy level of an electron within an atom. According to quantum mechanics, every principal energy level has one or more sub-levels within it. The number of sub-levels in a given energy level is equal to the number assigned to that energy level. That is, principal energy level 1 will have 1 sub-level, principal energy level 2 will have two sub-levels, principal energy level 3 will have three sub-levels, and so on. In any energy level, the maximum number of electrons possible is $2n^2$. Therefore, the maximum number of electrons that can occupy the first energy level is 2 $(2 \cdot 1^2)$. For energy level 2, the maximum number of electrons is 8 $(2 \cdot 2^2)$, and for the 3rd energy level, the maximum number of electrons is 18 $(2 \cdot 3^2)$. **Table** 1.1 lists the number of sub-levels and electrons for the first four principal quantum numbers.

TABLE 1.1: Number of Sub-levels and Electrons by Principal Quantum Number

Principal Quantum Number	Number of Sub-Levels	Total Number of Electrons
1	1	2
2	2	8
3	3	18
4	4	32

The largest known atom contains slightly more than 100 electrons. Quantum mechanics sets no limit as to how many energy levels exist, but no more than 7 principal energy levels are needed to describe the electrons of all known atoms. Each energy level can have as many sub-levels as the principal quantum number, as discussed above, and each sub-level is identified by a letter. Beginning with the lowest energy sub-level, the sub-levels are identified by the letters *s*, *p*, *d*, *f*, *g*, *h*, *i*, and so on. Every energy level will have an *s* sub-level, but only energy levels 2 and above will have *p* sub-levels. Similarly, *d* sub-levels occur in energy level 3 and above, and *f* sub-levels occur in energy level 4 and above. Energy level 5 could have a fifth sub-energy level named *g*, but all the known atoms can have their electrons described without ever using the *g* sub-level. Therefore, we often say there are only four sub-energy levels, although theoretically there can be more than four sub-levels. The principal energy levels and sub-levels are shown in the following diagram. The principal energy levels and sub-levels that we use to describe electrons are in red.

Energy Levels	Sub-Levels							
1	s							
2	s	p						
3	s	p	d					
4	s	p	d	f				
5	s	p	d	f	g			
6	s	p	d	f	g	h		
7	s	p	d	f	g	h	i	
8	s	p	d	f	g	h	i	j

Orbitals

Quantum mechanics also tells us how many orbitals are in each sub-level. In Bohr's model, an orbit was a circular path that the electron followed around the nucleus. In quantum mechanics, an orbital is defined as an area in the electron cloud where the probability of finding the electron is high. The number of orbitals in an energy level is equal to the square of the principal quantum number. Hence, energy level 1 will have 1 orbital (1^2), energy level 2 will have 4 orbitals (2^2), energy level 3 will have 9 orbitals (3^2), and energy level 4 will have 16 orbitals (4^2).

The *s* sub-level has only one orbital. Each of the *p* sub-levels has three orbitals. The *d* sub-levels have five orbitals, and the *f* sub-levels have seven orbitals. If we wished to assign the number of orbitals to the unused sub-levels, *g* would have nine orbitals and *h* would have eleven. You might note that the number of orbitals in the sub-levels increases by odd numbers (1, 3, 5, 7, 9, 11, . . .).

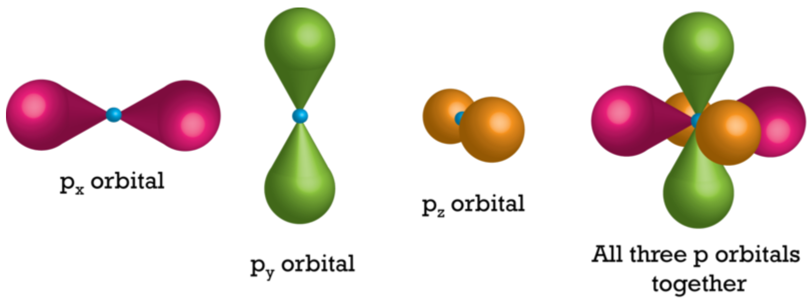
As a result, the single orbital in energy level 1 is the *s* orbital. The four orbitals in energy level 2 are a single 2*s* orbital and three 2*p* orbitals. The nine orbitals in energy level 3 are a single 3*s* orbital, three 3*p* orbitals, and five 3*d* orbitals. The sixteen orbitals in energy level 4 are a the single 4*s* orbital, three 4*p* orbitals, five 4*d* orbitals, and seven 4*f* orbitals.

Principal Energy Level (n)	Number of Orbitals Present s	p	d	f	Total Number of Orbitals (n^2)	Maximum Number of Electrons ($2n^2$)
1	1	-	-	-	1	2
2	1	3	-	-	4	8
3	1	3	5	-	9	18
4	1	3	5	7	16	32

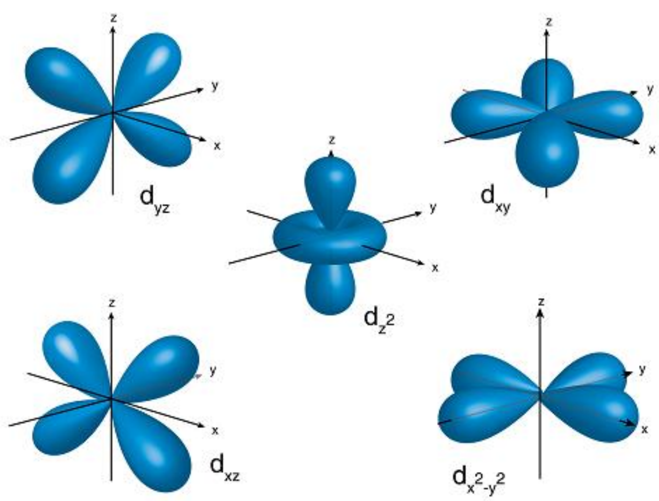
The chart above shows the relationship between *n* (the principal quantum number), the number of orbitals, and the maximum number of electrons in a principal energy level. Theoretically, the number of orbitals and number of electrons continue to increase for higher values of *n*. However, no atom actually has more than 32 electron in any of its principal levels.

Each orbital will also have a probability pattern that is determined by interpreting Schrödinger's equation. Earlier, we showed that the probability pattern for an atom with a single electron is a circle. The illustration, however, is 2-dimensional. The real 3-dimensional probability pattern for the single orbital in the *s* sub-level is actually a sphere.

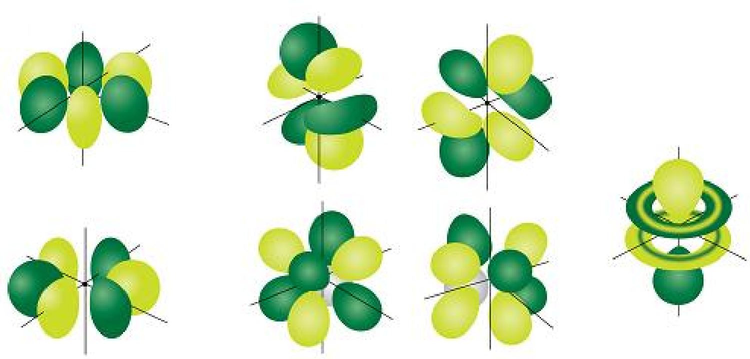
The probability patterns for the three orbitals in the *p* sub-levels are shown below. The three images on the left show the probability pattern for the three *p* orbitals in each of the three dimensions. On the far right is an image of all three *p* orbitals together. These *p* orbitals are said to be shaped like dumbbells (named after the objects weight lifters use), water wings (named after the floating balloons young children use in the swimming pool), and various other objects.



The probability patterns for the five *d* orbitals are more complicated and are shown below.

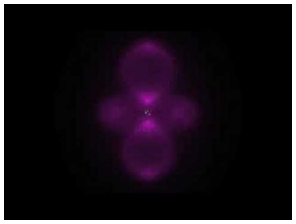


The seven **f** orbitals shown below are even more complicated.



You should keep in mind that no matter how complicated the probability pattern is, each shape represents a single orbital, and the entire probability pattern is the result of the various positions that either one or two electrons can take.

A video discussing the relationship between spectral lines and electron transitions is available at **(1j)** http://www.youtube.com/watch?v=fKYso97eJs4 (3:49).



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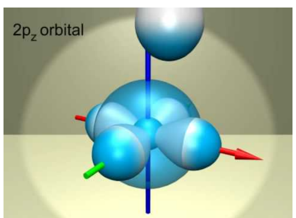
A short animation of s and p orbitals is available on youtube.com at http://www.youtube.com/watch?v=VfBcfYR1VQo (1:20).



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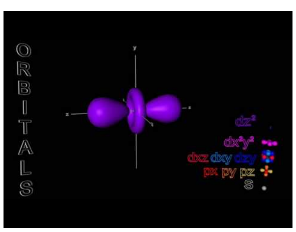
Another example of s, p and d electron orbitals is available also on youtube.com at http://www.youtube.com/watch?v=K-jNgq16jEY (1:37).



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Lesson Summary

- Solutions to Schrodinger's equation involve four special numbers called quantum numbers, which completely describe the energy of an electron.
- Each electron has exactly four quantum numbers.
- According to the Pauli Exclusion Principle, no two electrons have the same four quantum numbers.
- The major energy levels are numbered by positive integers (1, 2, 3, ... , n), and this number is called the principal quantum number
- Quantum mechanics also tells us how many orbitals are in each sub-level.
- In quantum mechanics, an orbital is defined as an area in the electron cloud where the probability of finding the electron is high.

Further Reading / Supplemental Links

The following is a video on the quantum mechanical model of the atom.

- http://www.youtube.com/watch?v=IsA_oIXdF_8&feature=related

This video is a ChemStudy film called "Hydrogen Atom and Quantum Mechanics." The film is somewhat dated but the information is accurate. The video also contains some data supporting quantum theory.

- http://www.youtube.com/watch?v=80ZPe80fM9U

Review Questions

1. How many sub-levels may be present in principal energy level 3 ($n = 3$)?
2. How many sub-levels may be present in principal energy level 6 ($n = 6$)?
3. Describe the difference in the definitions of a Bohr orbital and a quantum mechanics orbital.
4. What is the maximum total number of electrons that can be present in an atom having three principal energy levels?

In the first image of this chapter, the photograph showing water waves diffracting through a gap between small rocks is from http://www.flickr.com/photos/framesof mind/554402976/ (CC-BY-SA).