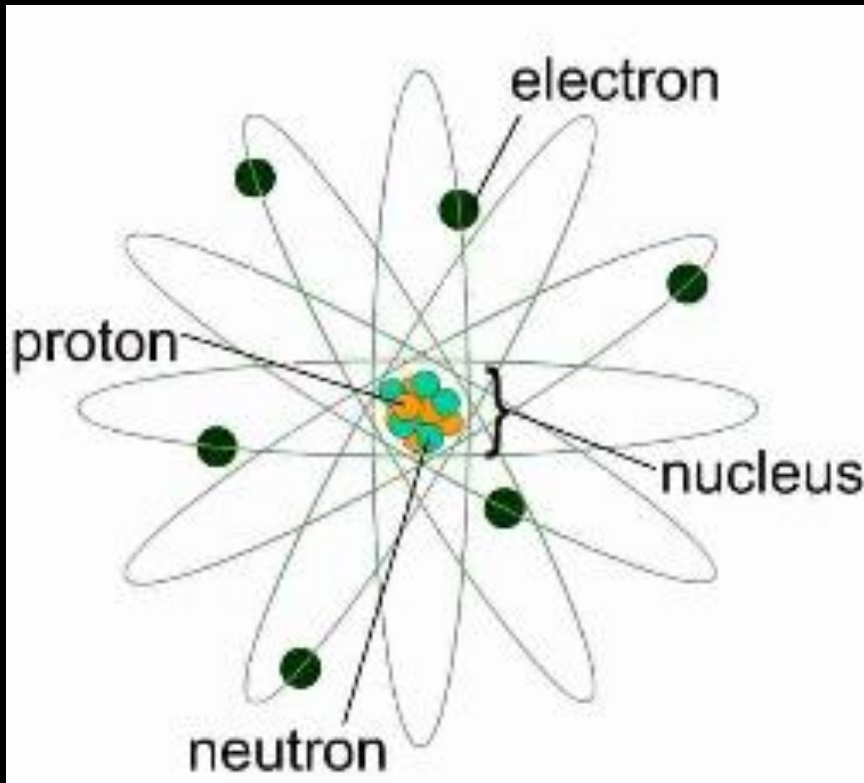




QUANTUM CHEMISTRY

REMEMBER THE ATOM...



- Protons have a charge of +1 and a mass of 1.
- Neutrons have no charge and a mass of 1. Protons and neutrons make up the nucleus.
- Electrons have a charge of -1 and a mass of $1/1837$. They are found around the nucleus, confined to specific regions of space known as orbitals.

ENERGY LEVEL

- Orbitals are 3-dimensional regions of space around a nucleus in which electrons are likely to be found.
- Bohr's discovery of the energy levels was later refined and is now known as the principle quantum number or shell.
- These energy levels (or shells) are assigned whole numbers (1, 2, 3, 4...).
- The term energy level reminds us that this simply describes the average energy of electrons found within that shell.
- The main categories of orbitals correspond to the various energy levels around the nucleus, which the electrons can occupy.

ORBITS AND ORBITALS

- Orbits refer to specific *paths* around an object, like the orbit of the Earth around the Sun.
- Orbitals refer to *regions* of space.
- Electrons **do NOT** travel in orbits, but rather are located in orbitals.
- Rutherford established that electrons are located around the nucleus, and Bohr determined that they travel in paths in various levels
- The chemists and physicists who developed quantum mechanics (also called wave mechanics) established that electrons are located in orbitals; they also found that the electrons are governed by several other quantum numbers

NUMBER OF ORBITALS

- The maximum number of orbitals that can be in each energy level is given by the formula:

$$\# \text{ orbitals} = n^2$$

where n = energy level

- The maximum number of electrons that can be in each energy level is given by the formula:

$$e = 2n^2$$

where e = electrons
 n = energy level

ENERGY LEVELS, ORBITALS AND ELECTRONS

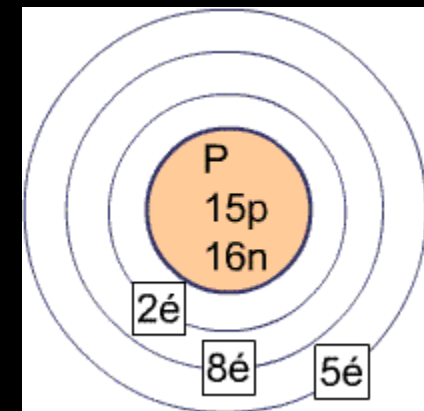
Energy Level (n)	Number of orbitals (n^2)	Number of electrons ($2n^2$)
1	$n^2=1$	2
2	$n^2=4$	8
3	$n^2=9$	18
4	$n^2=16$	32
...

Example

Consider the phosphorus atom.

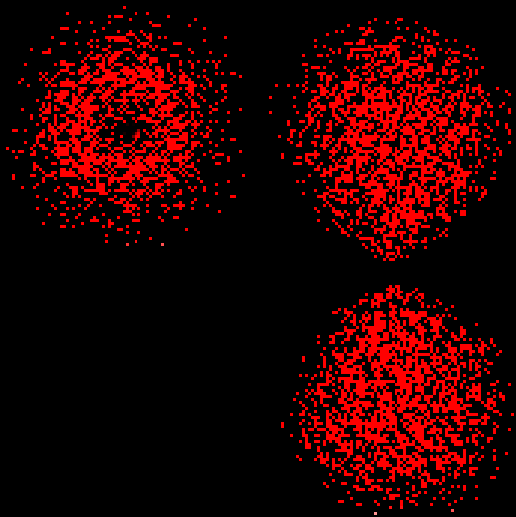
Its atomic number of 15, so it has 15 electrons and 15 protons.

Its atomic mass is 31, which means that it has $31-15=16$ neutrons.

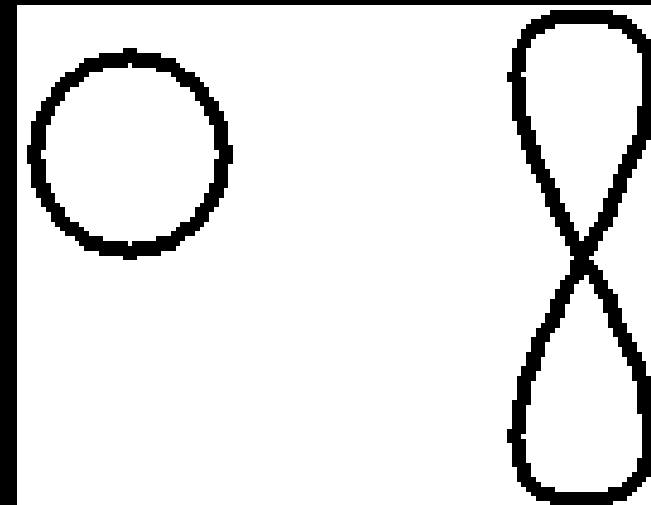


HEISENBERG'S UNCERTAINTY PRINCIPLE

- In 1926, Werner Heisenberg (1901-1976) formulated **Heisenberg's uncertainty principle**
 - an electron's location and velocity around an atom's nucleus at a given time cannot both be determined precisely. A cloud of probability is used to represent where the electrons are most likely to be found.



To simplify you can represent the orbitals with lines instead of the “speckled” areas.



QUANTUM NUMBERS

- **Quantum Numbers**
- Each electron orbital of the atom may be described by a set of four quantum numbers. They give the position with respect to the nucleus, the shape of the orbital, its special orientation and the spin of the electron in the orbital.
- **Principal quantum number (n)**
- Refers to the average distance of the orbital from the nucleus. They are the energy levels or shells.
- **Secondary quantum number (azimuthal quantum number) (l)**
- Refers to the shape of the orbital. It is also referred to as the angular momentum quantum number. This number controls the number of subshells within a particular energy level.

SPIN AND PAULI EXCLUSION PRINCIPLE

- **Magnetic quantum number (m_l)**
- Refers to the number of special orientations of orbitals in space.
- **Spin quantum number (m_s)**
- Describes the spin in either of two possible directions. Each orbital can be filled by only two electrons, each with an opposite spin.
- The main significance of electron spin is explained by the postulate of Wolfgang Pauli (1900-1958). It states that in a given atom, no 2 electrons can occupy the same quantum state (therefore they cannot have the same set of 4 quantum numbers (n , l , m_l and m_s)). This is referred to as the **Pauli exclusion principle**.

n	l	Orbital designation	m_l	# of orbitals	# electrons per orbital	# electrons per energy level
1	0	1s	0	1	2	2
2	0	2s	0	1	2	8
	1	2p	-1,0,+1	3	6	
3	0	3s	0	1	2	18
	1	3p	-1,0,+1	3	6	
	2	3d	-2,-1,0,+1,+2	5	10	
4	0	4s	0	1	2	32
	1	4p	-1,0,+1	3	6	
	2	4d	-2,-1,0,+1,+2	5	10	
	3	4f	-3,-2,-1,0,+1,+2,+3	7	14	

PAGES...

- Copy out the figure 3.14 into your notes (page 177)
- Page 179 Questions 1-10