Shapes of Molecules & Carbon Allotropes

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Special thanks to Ms Williams and Ms Matrella for their constant support and inspiration

Please note that these guides are a collation of my personal notes, teachers' notes, chemistry books, and websites such as chemguide, chemsheets, chemwiki and wikipedia.

Valence-Shell Electron-Pair Repulsion Theory

A covalent molecule will have a shape, which is determined by the angels between the bonds joining the atoms together. The arrangement of electrons pairs around the central atom in a molecule depends on the number of electron pairs. These pairs have a repulsion between them and want to be as far apart from each other as possible and hence cause the least repulsion. There are 2 types of electron pairs:

- Bonding Pairs: are being shared between the central atom and a bonded one.
- Lone Pairs: are attached to the central atom only.

The repulsion between these pairs isn't equal though. The greatest repulsion occurs between 2 lone pairs, then a lone and a bonded pair and the least repulsive of them is between 2 bonded pairs. This difference in repulsive forces is what leads to a variety of shapes in molecules.

Determining the Shape

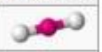
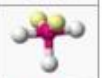
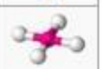
Molecules

Below is a table showing some possible shapes (and bond angles) of molecules with up to 6 electron pairs around its central atom. But how is the number of electron pairs determined? Let's take BF_3 as an example. Boron has 3 valence electrons and each Fluorine would share an electron each. Hence Boron now has 6 valence electrons. This is equivalent to 3 electron pairs. All of those pairs would be used to bond Boron with the 3 Fluorines. Hence the shape will be a trigonal planar and the bond angles will be 120 degrees.

Another example would be SF_6. Sulphur has 6 valence electrons and 6 Fluorines would share an electron each. The central atom S would hence have 6 e^- pairs, all of which are bonding resulting in an octahedral molecule with the angles mentioned above.

This sort of calculation can be applied to quite a lot of molecules, however when we want to figure out the shape of an ion the procedure is tweaked.

From *Wikipedia* (ignore the example's bond angle):

Bonding electron pairs	Lone pairs	Shape	Ideal bond angle (example's bond angle)	Example	Image
2	0	linear	180°	CO_2	
3	0	trigonal planar	120°	BF_3	
2	1	bent	120° (119°)	SO_2	
4	0	tetrahedral	109.5°	CH_4	
3	1	trigonal pyramidal	107°	NH_3	
2	2	angular	109.5° (104.5°)	H_2O	
5	0	trigonal bipyramidal	90°, 120°, 180°	PCl_5	
4	1	seesaw	180°, 120°, 90° (173.1°, 101.6°)	SF_4	
3	2	T-shaped	90°, 180° (87.5°, $<$ 180°)	ClF_3	
2	3	linear	180°	XeF_2	
6	0	octahedral	90°, 180°	SF_6	
5	1	square pyramidal	90° (84.8°), 180°	BrF_5	
4	2	square planar	90°, 180°	XeF_4	

Polyatomic Ions

When we have an ion such as Ammonium, NH_4^+ we do the following:

N has 5 valence e^-

4 Hydrogens share 4 e^-

the +1 charge means we take away 1 e^- from the total electrons around the central atom. (if this was a negative sign we add it on to our total)

Hence the central atom has 4 electron pairs in this case, all of which are bonded. We can flick back to the table to see that NH_4^+ has a tetrahedral structure with a 109.5 bond angle.

Spec. Compounds

The spec mentions only these compounds to be memorised, the angles are in the brackets

- $BeCl_2$ = LINEAR (180)
- BCl_2 = TRIGONAL PLANAR (120)
- CH_4 = TETRAHEDRAL (109.5)
- NH_4^+ = TETRAHEDRAL (109.5)
- NH_3 = TRIGONAL PYRAMIDAL (107)
- H_2O = BENT/ V SHAPED (104)
- CO_2 = LINEAR (180)
- Gaseous PCl_5 = TRIGONAL BIPYRAMID (90, 120)
- SF_6 = OCTAHEDRAL (90)

Bond Length

Bond length measures the distance between the two nuclei in a covalent bond. The important thing about bond length is its relationship with bond energy.

In a covalent bond, the two atoms are held together because both nuclei are attracted to the same pair of electrons. In a longer bond, the shared electron pair is further from at least one of the two nuclei, and so the attractions are weaker.

Carbon Allotropes

No need to memorise chunks of text in this section, just have a read

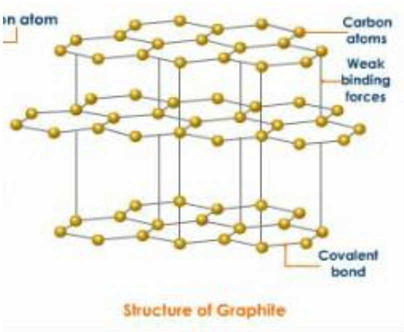
Allotropes are different forms of an element that exist in the same physical state. Here are some of Carbon allotropes:

Diamond:

- Each C atom is bonded to 4 other C atoms resulting in an interlocking tetrahedral structure, i.e. a macromolecule.
- The hardest substance on the planet, hence used for drilling and cutting
- A poor conductor and hence a really good insulator
- Diamonds used in industrial applications are made artificially under very high temp and pressure). This is to save money or else too much will be spent on mining natural diamonds and no profits will be made.

Graphite:

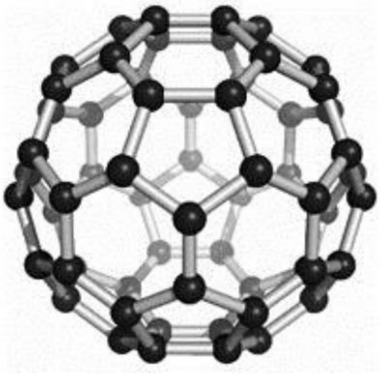
- Occurs naturally but can also be manufactured from amorphous carbon (will be discussed later)
- A very good conductor of both heat and electricity
- Chemically inert, hence used as an electrode in electrolysis
- Consists of planes of trigonal carbon atoms arranged in sheets held together by weak forces called Van der Waals



Amorphous Carbon

- Carbon atoms with an irregular shape
- Occurs naturally as soot or coal (black powder basically)
- Can be manufactured by heating organic material to very high temperatures in absence of air
- Buns easily in air

- Used as filler for rubber and plastics and black pigment, as well as fuel (coke and coal)



Fullerenes

- Spherical carbon allotropes made up of varying numbers of carbon atoms are called fullerenes
- Discovered in 1985 and nicknamed buckyball
- Buckminsterfullerene is made from 20 hexagons and 12 pentagons, total 60 Carbon atoms
- It is a black solid that dissolved in petrol to give a deep red solution
- Contains delocalised electrons hence can conduct electricity
- Used medically to deliver a drug into body cells without "leaking" on the way
- Bond angle is not 120^0 between carbon bonds
- Note that fullerenes are NOT considered giant covalent structures.

Nanotubes

- Discovered in 1991 by a Japanese scientist
- They are a new type of fullerene made up of cage-like tubes of carbon atoms
- Fullerene nanotubes are not the same as nanoparticles, they are small molecular carbon tubes. They are called nanotubes because they have applications in nanotechnology due to their molecular structure
- Nanotubes can be 12 times stronger than steel and already used in tennis racquets and car bodies
- Some nanotubes are superconducting (zero resistance to electric currents).
- Large surface area of fullerenes means they have potential use as catalysts.
- They can be/are being used in the military and in the space industry.
- These properties can cause a revolution in electrical, chemical, mechanical and civil engineering, however since they were discovered so recently we still don't know much about their disadvantages or long term effects and hence we should research more about them before scaling their usage to consumer level across the globe.