

4 THE SHAPE OF MOLECULES

In senior high school chemistry, the constitution of a substance was expressed in a structural formula printed on a page using symbols for elements and bonds. The concept of asymmetric carbon atoms was taught to some extent, but only as exceptional cases. In general, the structures were treated as though they were planar.

In university chemistry, the structure of a substance is regarded as three-dimensional, and planar molecules as exceptional. Furthermore, you learn the factors that determine the three-dimensional structure of substance.

This chapter will discuss the structures of some representative inorganic and organic compounds as examples. It is essential for you to learn stereochemistry in order to understand the central problem of modern chemistry, the relation between structure and function of a molecule.

4.1 Structures of simple compounds

Ionic bonds are formed by the electrostatic attraction between a cation and an anion. Since the electric field of an ion has spherical symmetry, ionic bonds have no directional character. On the other hand, covalent bonds are formed by the overlap of atomic orbitals. Since the overlap is such that the atomic orbitals can attain maximum overlap, a covalent bond necessarily has a directional character. Hence, the shape of a molecule is determined by the angle between two bonds, which in return is determined by the atomic orbitals that form the bond.

The above is a general discussion concerning the molecular structure. The structure of simple molecules can be inferred by a simple stereochemical consideration which will be explained.

(a) Valence shell electron pair repulsion theory

In 1940, Sidgwick proposed a theory called valence shell electron pair repulsion (VSEPR) theory, which being qualitative, is very easy to understand. The theory is suitable for predicting the structure of XY_m type compounds. According to this theory, the number of electron pairs determines the arrangement of these pairs around the central atom of the molecule. There is electrostatic repulsion between any two electron pairs that tends to push apart the atomic orbitals as far as possible. Since an electron pair occupies an atomic orbital, a lone pair has also the same effect as that of a bonding electron pair. In other words, a lone pair and a bonding electron pair also repel each other and separate them as far as possible.

Compounds with a divalent central atom

According to the VSEPR theory, two electron pairs belonging to a divalent central atom will be most widely separated when the bond angle is 180° . In other words, the molecule will have a linear structure. In fact, beryllium chloride $BeCl_2$, with a divalent central atom, is a linear molecule. As will be described later, some compounds such as carbon dioxide $O=C=O$ and allene $H_2C=C=CH_2$ are also linear as though these have a divalent central atom.

Compounds with a trivalent central atom

If the VSEPR theory is applicable to compounds with a trivalent central atom such as boron trichloride BCl_3 , the bond angle $\angle Cl-B-Cl$ should be 120° with the four atoms in the same plane. A similar trigonal planar structure is observed for stannic chloride, $SnCl_4$.

Do notice that a similar triangular structure is observed for ethylene $H_2C=CH_2$, the nitrate ion NO_3^- and sulfur dioxide SO_2 .

Compounds with a tetravalent central atom

The theory of tetrahedral carbon as proposed by the Dutch chemist Jacobus Henricus van't Hoff (1852-1911) and the French chemist Joseph Achille Le Bel (1847-1930), who reached the theory nearly at the same time, can also be derived automatically from the VSEPR theory. As for methane,

the structure in which the repulsion among four electron pairs is minimal is not a square with bond angles of 90° but a tetrahedron with bond angles of 109.5° , definitely larger than 90° .

Interestingly, ammonium ion NH_4^+ with nitrogen as the central atom is also tetrahedral like methane. If the lone pair is counted, the nitrogen atom of ammonia NH_3 and the oxygen atom of water H_2O may be regarded tetravalent. These are not rigidly tetrahedral, and the bond angle $\angle\text{H-N-H}$ is 106° and $\angle\text{H-O-H}$ is 104.5° . These facts suggest the following qualitative relation.

The relative magnitudes of repulsion

lone pair-lone pair > lone pair-shared electron pair > shared electron pair-shared electron pair

Some polyatomic ions such as SO_4^{2-} and SO_3^{2-} have a tetrahedral structure.

Compounds whose central atom has a valency higher than four

The structure of compounds whose central atom has a valency higher than four can also be explained in terms of the VSEPR theory. A pentavalent compound has a trigonal bipyramidal structure. A representative compound of this type is phosphorous pentachloride PCl_5 . A compound with a hexavalent central atom is octahedral, which is in fact a square bipyramid. A good example is sulfur hexafluoride SF_6 . In the case of a heptavalent compound, the situation is the same and its structure is a pentagonal bipyramid.

Compounds must be considered in which a lone pair acts the role of a shared electron pair. For instance, IF_5 and ICl_4 are compounds of this type. In Fig. 4.1 the structures of such compounds are shown.

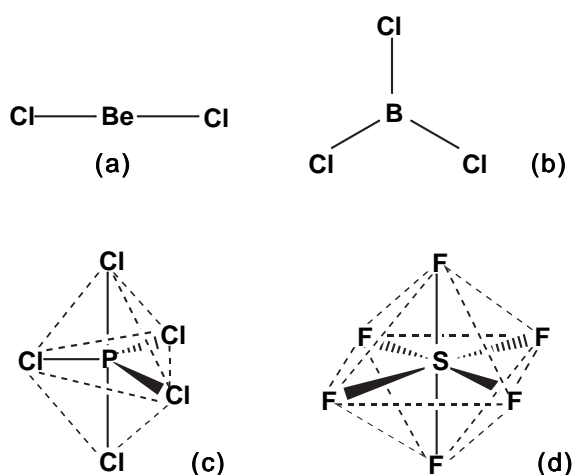


Figure 4.1 The structure of typical inorganic compounds

(a) linear BeCl_2 ; (b) trigonal BCl_3 ;

(c) trigonal bipyramid PCl_5 ; (d) octahedron SF_6

Sample exercise 4.1 Prediction of structures based on the VSEPR theory

Predict the structures of the chemical species given below based on the VSEPR theory.

(a) SO_2 , (b) SO_3 (c) SO_4^{2-}

Answer

(a) triangle, (b) tetrahedral (approximately), (c) tetrahedral

(b) Hybridization of atomic orbitals

It is expected that beryllium chloride BeCl_2 and tin(II) chloride SnCl_2 will have a similar structure since these have similar molecular formulas. However, the former has a linear structure,

while the latter has a bent structure. This can be explained by the difference in the atomic orbitals that are employed. When electrons occupy the atomic orbitals following the Aufbau principle, electrons will fill the atomic orbital of the lowest energy. Two electrons are allowed to occupy one orbital. According to the Pauli exclusion principle, there are no electrons with the same set of quantum numbers (Ch. 2.4 (d)). A problem arises as to which orbitals the fourth electron of the carbon atom should occupy. It is established that the lowest energy configuration for an atom is the one having the maximum number of unpaired electrons allowed by the Pauli principle in a set of orbitals with the same energy (in this case three 2p orbitals). In that case all first electrons have the same spin magnetic quantum number (*i.e.*, $+1/2$ or $-1/2$) (Fig. 4.2).

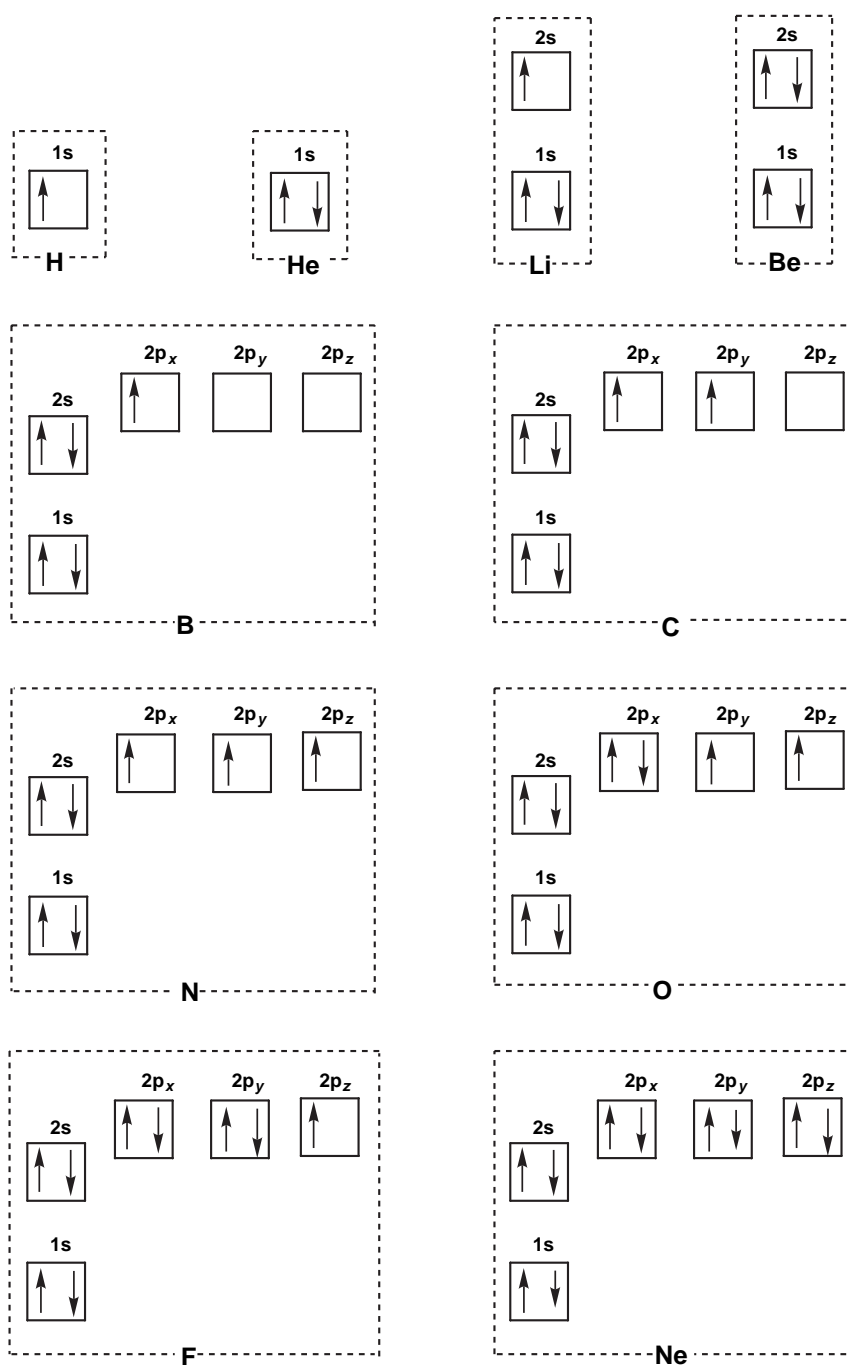


Figure 4.2 Electron configurations of atoms; from hydrogen to neon. The orbitals are progressively occupied in the manner described below.

Beryllium has two valence electrons and its electron configuration is $(1s^2 2s^2)$. In order for the

beryllium atom to form bonds as a divalent atom, the 2s and 2p atomic orbitals must form a pair of sp hybridized orbitals. Since two sp hybridized orbitals form the bond angle of 180° , BeCl_2 is necessarily linear.

Similarly boron has three valence electrons and its electron configuration is $(1s^2 2s^2 2p^1)$; hereafter simply $1s^2 2s^2 2p$). In order to form bonds as a trivalent atom, the electron configuration should be $(1s^2 2s 2p_x 2p_y)$. One 2s and two 2p orbitals will make three sp^2 hybridized orbitals. Since the angle between two sp^2 hybridized orbitals is 120° , BCl_3 is necessarily a triangle.

In the case of carbon compounds, their structures can be explained if one assumes that four equivalent sp^3 orbitals are formed from one 2s and three 2p orbitals. A carbon atom has four valence electrons, and the electron configuration is $(1s^2 2s^2 2p^2)$, and to form bonds as a tetravalent atom, the electron configuration must change into $(1s^2 2s 2p_x 2p_y 2p_z)$. By hybridization, four equivalent sp^3 hybridized orbitals are formed. The bond angle made by two sp^3 hybridized orbitals is 109.5° (tetrahedral angle). This is the reason why methane is tetrahedral.

In the case of nitrogen compounds, ammonia NH_3 for instance, four out of five valence electrons of a nitrogen atom will occupy the four sp^3 hybridized orbitals as shown in Fig. 4.3. The remaining one valence electron will occupy one of the hybridized orbitals which have already one electron. Hence the spin of the second electron must be opposite to that of the first electron. Consequently the nitrogen atom will be trivalent with one lone pair.

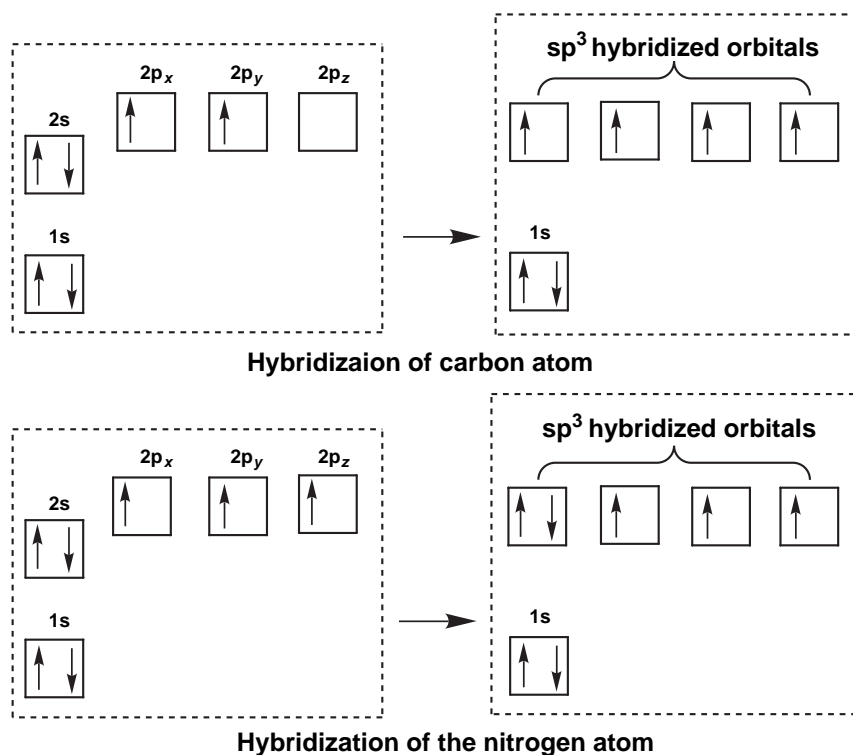


Figure 4.3 Hybridization.

Hybridization of the atomic orbitals of carbon and nitrogen atoms

In the case of phosphorus, there are two cases. In one case the atom is trivalent with one lone pair as is the case for nitrogen, and in the other case phosphorus is pentavalent with a dsp^3 hybridized orbital. Pentavalent phosphorous has a trigonal bipyramidal structure. Complex ions with cobalt or nickel ions as the central atom are hexacoordinated with octahedral structure.

As discussed above, both the VSEPR theory and the hybridization of atomic orbitals give the same conclusion on the structure of molecules and ions. Though the VSEPR theory depended solely on the repulsion between electron pairs, the theory of hybridization gave some theoretical justification.

4.2 The structures of carbon compounds

(a) Isomerism due to the asymmetric carbon atom; optical isomerism

Before the theory of valence was established, the French chemist/physiologist Louis Pasteur (1822-1895) had already comprehended the effect of the structure of individual molecules on the properties of an assembly of molecules. He successfully separated racemic acid (in fact its ammonium sodium salt) into (+)- and (-)-**tartaric acid** based on the difference in the direction of the hemihedral faces of their crystals (1848).

The two compounds have the same physical and chemical properties (*e.g.*, m.p.), but there is a difference in the optical properties in solutions of each compound. Both rotated the polarized plane; in other words, both had **optical activity**. However, the **specific rotations** of the two compounds, which are a measure of the rotating power of the compound in question, had the same absolute value but the signs were reversed. Since molecules exist separately in solution, the difference could not be attributed to the difference in their crystal structures. Unfortunately, at that time the atomic theory was accepted but the theory of valence had not yet been introduced. Under such circumstances even Pasteur could not give a proper explanation for his discoveries.

In 1860s, the German chemist Johannes Adolf Wislicenus (1835-1902) found that the two kinds of lactic acids known at that time were both α -hydroxypropanoic acid $\text{CH}_3\text{CH}(\text{OH})\text{COOH}$, not β -hydroxypropanoic acid $\text{HOCH}_2\text{CH}_2\text{COOH}$. He further suggested that a novel concept for stereoisomers should be introduced to explain this phenomenon. The new concept stated that two compounds that have the same structural formula in two dimensions could be stereoisomers if the spatial arrangement of the atoms was different.

In 1874, van't Hoff and Le Bel independently proposed the theory of the tetrahedral carbon atom. According to this theory, the two lactic acids may be drawn as shown in Fig. 4.4. The one lactic acid is the mirror image of the other. In other words, the two compounds were related as with left and right hands, and hence they may be called **antipodes** or **enantiomers**. Thanks to the theory of van't Hoff and Le Bel, the new field of chemistry, **stereochemistry**, rapidly developed.

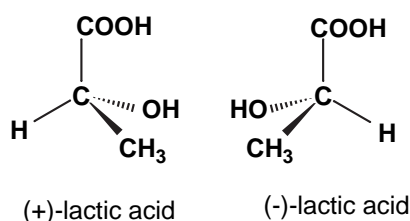
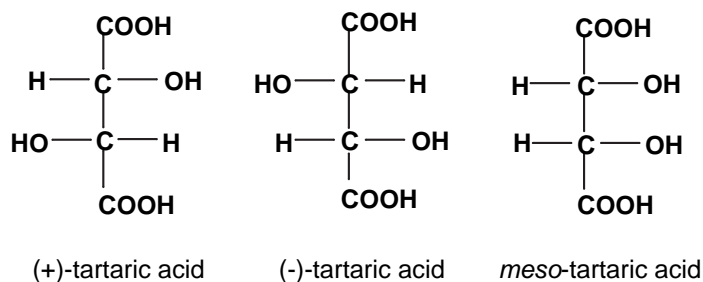


Figure 4.4 Stereoisomers of lactic acids.

The two isomers are antipodes, that is, have a relation of left and right hands.

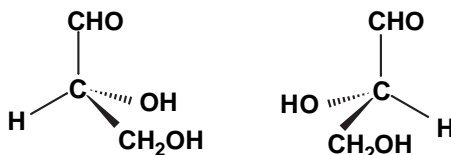
To the central atom of lactic acid, four different atoms or groups of atoms are bonded. Such a carbon atom is called the **asymmetric carbon atom**. Generally speaking, the number of stereoisomers will be 2^n , n being the number of asymmetric carbon atoms. Tartaric acid has two asymmetric carbon atoms. However, because of the presence of symmetry in the molecule, the number of isomers is less than 2^n , and moreover one of the stereoisomers is optically inactive (Fig. 4.5). All these phenomena can be consistently explained by the theory of the tetrahedral carbon atom.

**Figure 4.5** Stereoisomers of tartaric acid

(+)-tartaric acid and (-)-tartaric acid form an enantiomeric pair. Because of the presence of symmetry, however, *meso*-tartaric acid is optically inactive.

Sample exercise 4.2 Glyceraldehyde

Draw the perspective view of glyceraldehydes $\text{OHCCHOHCH}_2\text{OH}$, the simplest sugar, in the manner shown in Fig. 4.4.

Answer

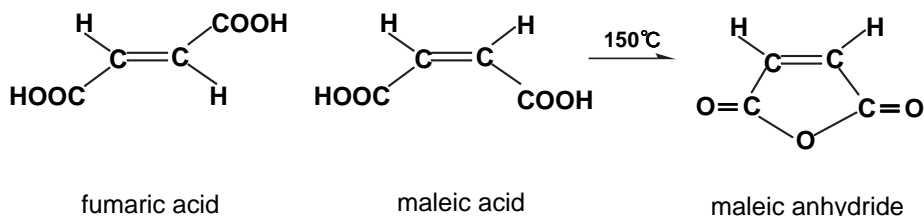
Note that there are many other ways of drawing.

(b) Geometrical isomers

Van't Hoff explained that the isomerism of fumaric and maleic acids was due to the restricted rotation about a double bond, an explanation different from that for optical isomerism. This type of isomerism is called **geometrical isomerism**. In the ***trans* form** the substituents (in the case of fumaric and maleic acids, the carboxy group) are located on different sides of the double bond, while in the ***cis*-form** the substituents are located on the same side.

Of the two isolated isomers, van't Hoff assigned the one that readily lost a molecule of water to turn into maleic anhydride to the *cis*-isomer because in the *cis*-isomer the two carboxy groups are close together. By heating up to 300°C , fumaric acid was converted to maleic anhydride. This is reasonable since the process should involve a *cis-trans* isomerization which is a process with a considerably high energy barrier (Fig. 4.6).

Since several pairs of geometrical isomers were already known, the theory of geometrical isomerism offered good support for the structural theory of van't Hoff.

**Figure 4.6** Geometrical isomers

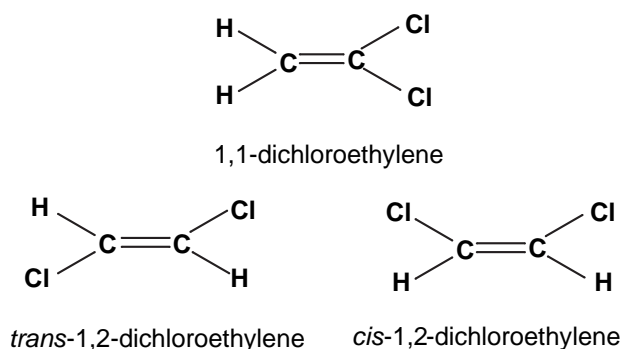
Maleic acid (*cis*-form) has two carboxy groups which are close together, and hence readily lose a molecule of water to give acid anhydride (maleic anhydride).

Sample exercise 4.3 Isomers of dichloroethylene

Draw the structural formula of all isomers of dichloroethylene $\text{C}_2\text{H}_2\text{Cl}_2$.

Answer

The two chlorine atoms may bond to the same carbon atom, or to different carbon atoms. There is geometrical isomerism in the latter case.



(c) The structure of benzene

The structure of benzene had been an enigma for many years. In 1865, Kekulé proposed a planar cyclic structure where three single and three double bonds were alternatively connected. The structure was called the **Kekulé structure**. The evidence for such a structure was essentially the number of substituted benzene isomers. With the Kekulé structure, there should be three isomers for cresol, *i.e.*, *o*-, *m*- and *p*-cresol (Fig. 4.7).

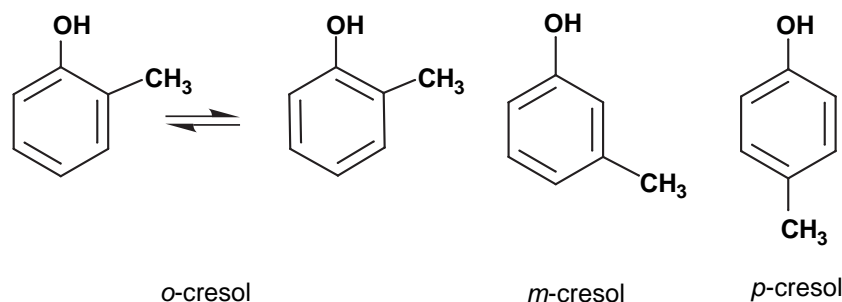


Figure 4.7 Isomers of cresol.

There are three isomers, *o*-, *m*-, and *p*-cresol depending on the location of the substituents (CH_3 and OH). There are two isomers for *o*-cresol.

The Kekulé structure could not solve all problems concerning the structure of benzene. If benzene has the structure proposed by Kekulé, there should be two isomers for *o*-cresol, which was not the case. Kekulé postulated a rapid equilibrium, which was called resonance between the two structures. Later the idea of resonance was explained in terms of quantum mechanics.

(d) The structure of ethane: conformational analysis

The theory of the tetrahedral carbon atom and that of the structure of benzene gave a foundation for the theory of the structure of organic compounds. However, van't Hoff and other chemists recognized that there remained some problems that could not be explained in terms of the tetrahedral carbon theory. That was the isomerism caused by the rotation about a single bond.

If the rotation about the C-C bond in 1,2-dichloroethane $\text{CH}_2\text{ClCH}_2\text{Cl}$ is restricted as is the case with fumaric and maleic acids, there should be numerous isomers. Though van't Hoff considered such a possibility, he finally concluded that the rotation was free (**free rotation**) because no rotational isomers due to the restricted rotation were observed. He added that the observed structure was an average of all possible structures.

In the 1930s it was proved both by theory and experiment that the rotation about a single bond was not necessarily perfectly free. In the case of ethane, the repulsion between the hydrogen atoms bonded to the adjacent carbon atoms would form a barrier to free rotation, and the magnitude of the repulsion would vary with the C-C bond rotation. Fig. 4.8(a) is the Newman projection of ethane,

and Fig. 4.8(b) is the energy-torsion angle plot.

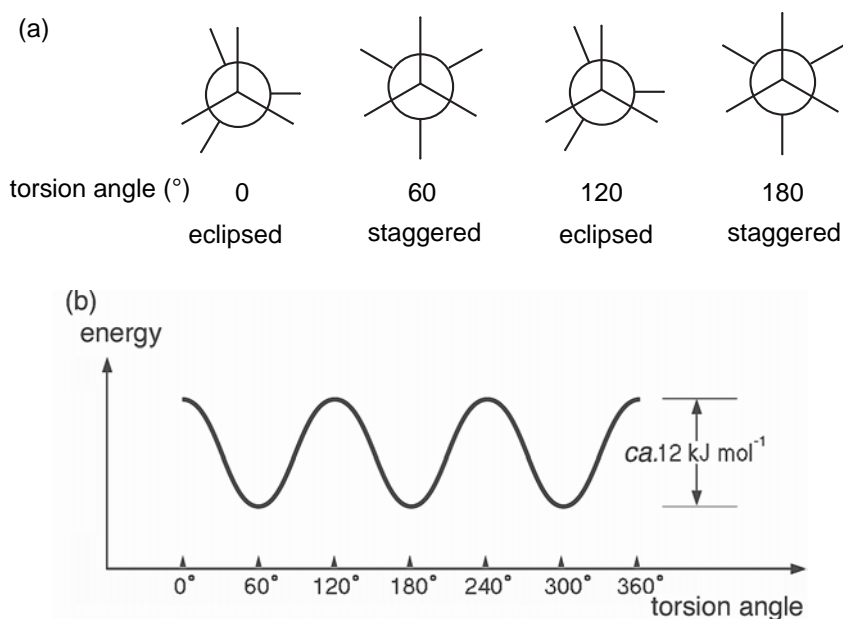


Figure 4.8 Conformational analysis of ethane

In the drawing (a) (Newman projection), you are supposed to observe the molecule from the direction of the C-C bond. The front carbon atom is represented by the cortex of three short lines (each representing a C-H bond) while a circle represents the rear carbon atom. The whole picture corresponds to a projection of the molecule on a wall behind. For simplicity's sake hydrogen atoms are not drawn. (b) When the torsion angle is 0° , 120° , 240° and 360° , the rear part of the molecule is eclipsed by the front part. If you draw the Newman projection in that way, you cannot see the rear part. By convention, the rear part is rotated a bit so that you can see it.

When the angle of rotation (*i.e.*, the torsion angle) is 0° , 60° , 120° and 180° , the energy of the molecule is either a maximum or a minimum. The structure (conformation) with the torsion angle of 0° or 120° is called the **eclipsed** form, and the conformation with the torsion angle of 60° or 180° is called the **staggered** form. The study of the change of molecular structure caused by the rotation about a single bond is called **conformational analysis**. This analysis made great progress from the 1950s until now.

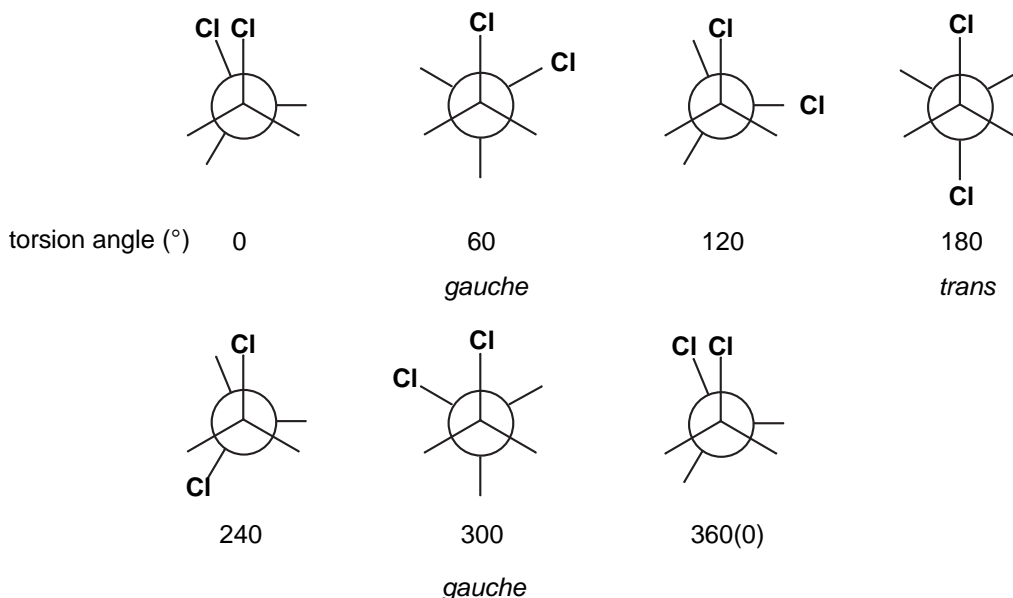
Conformational analysis of butane $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$ with respect to the central C-C bond, reveals that there are two staggered forms. The *trans* form, in which the two terminal methyl groups are on opposite sides, is $0.7 \text{ kcal mol}^{-1}$ more stable than the *gauche* isomer in which the two methyl groups are close to each other.

This result can be extended to such compounds as pentane and hexane which have additional methylene moieties, and finally to polyethylene which is made from innumerable bonded methylenes. In all of these, the all *trans* structure, *i.e.* the zigzag structure, is most stable. This is, however, valid only for solutions. For solid state substances other factors should be taken into consideration.

Sample Exercise 4.4 Conformational analysis of 1,2-dichloroethane

Portray the conformational analysis of 1,2-dichloroethane by rotating about C-C bond and draw the Newman projections as is shown in Fig. 4.8(a).

Answer



To summarize, the structure of carbon compounds is primarily determined by the hybridization state of the carbon atoms involved. When many conformations are possible by the rotation about a single bond, the most stable conformation will be chosen.

When the molecule has polar sites, other factors may be involved. An attractive interaction between positive and negative sites will make the structure with the larger steric hindrance more stable. In the case of salicylic acid, the hydrogen bond between the hydroxy and carboxy groups will make the more crowded structure more stable.

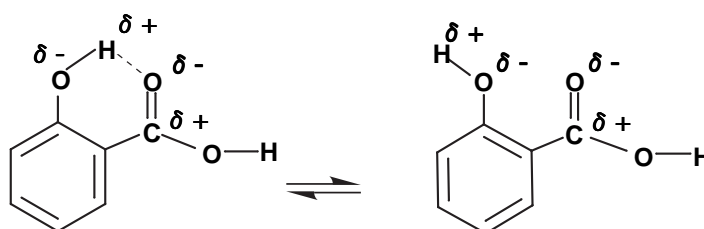


Figure 4.9 The hydrogen bond in salicylic acid.

Though the left structure involves more steric repulsion, the hydrogen bond makes it more stable.

In conclusion, the structure of carbon compounds can be reasonably explained if various factors are taken into consideration.

4.3 Structures of inorganic compounds

The structure of many simple inorganic compounds can be explained by the VSEPR theory or simple valence theory. However, some inorganic compounds which do not belong to this group are very important from both theoretical and practical viewpoints. Some of those compounds will be discussed below.

Ammonia

Ammonia NH_3 is derived from methane by replacing the carbon atom with a nitrogen atom and one of the hydrogen atoms with a lone pair. Thus, ammonia has a quasi-tetrahedral structure. However, to understand the structure of ammonia, you have to consider the **inversion** of the nitrogen atom. The behavior of ammonia is very similar to an umbrella that is blown inside out. The barrier to the inversion of ammonia is as low as $5.8 \text{ kcal mol}^{-1}$, and the inversion of ammonia at room temperature is very rapid (Fig. 4.10).

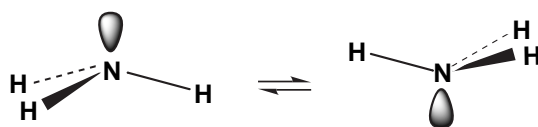


Figure 4.10 Inversion of ammonia

The behavior of the molecule is very similar to an umbrella that is blown inside out.

In principle, the nitrogen atom of an amine to which three different atoms or groups of atoms are bonded can be an asymmetric center because this nitrogen has four different substituents including a lone pair. Because of this inversion, however, this type of nitrogen atom cannot be an asymmetric center.

Diborane

It was expected that the reaction between magnesium boride and water would yield boron trihydride BH_3 . However, what was obtained is diborane B_2H_6 . Apparently this compound cannot be explained by simple valence theory, and a lot of effort has been spent to elucidate this anomaly.



It has been established that the compound has the strange structure shown below.

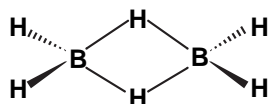


Figure 4.11 The structure of diborane.

The point is three-center, two-electron bond.

The skeleton of the molecule is a skewed quadrangle made by two boron and two hydrogen atoms, and the hydrogen atoms bonded to two boron atoms are called **bridged hydrogen**. The four terminal B-H bonds are normal in the sense that these are formed by the overlap of the 1s orbital of hydrogen and the hybridized orbital of boron. In contrast, the B---H---B bridge bond is a **three-center, two-electron bond** formed by hybridization of the 1s of hydrogen and the two hybridized orbitals of boron. The presence of such a bond is confirmed by quantum mechanics.

Rare gas compounds

It was long believed that rare gases exist only as monoatomic molecules, and do not form compounds. The Canadian chemist Neil Bartlett (1932-) obtained an ionic species $[\text{O}_2]^+[\text{PtF}_6]^-$ by the reaction between oxygen and platinum hexafluoride PtF_6 . He considered that much the same reaction should take place between xenon and PtF_6 since the 1st ionization energy of xenon is close to that of oxygen. In 1962 he in fact succeeded in obtaining the first rare gas compound $\text{Xe}(\text{PtF}_6)_x$, ($x = 1, 2$)

It became gradually apparent that rare gases form binary compounds with oxygen or fluorine which both have a high electronegativity. XeF_2 is a linear molecule with excess electrons while XeF_4 is the only square representative element compound. XeF_6 is a skewed octahedron, and in the vicinity of its melting point, it exists as crystalline $[\text{XeF}_5]^+\text{F}^-$.

Ferrocene

Ferrocene is composed of two cyclopentadiene rings which sandwich an Fe atom and is the first example of the group of compounds called **sandwich compounds** (Fig. 4.12).

In the early 1950s, a reaction between cyclopentadienylmagnesium bromide and anhydrous FeCl_3 was expected to yield fulvalene derivatives. However, a compound corresponding to

$(C_6H_5)_2Fe$ was obtained. The structure of this compound was found to be very unique: eighteen electrons, twelve from the two cyclopentadiene moieties (six electrons for each) and six outer shell electrons of Fe. Thus, it attains the electron configuration of a rare gas and comparable stability. The two cyclopentadiene rings rotate like musical discs.

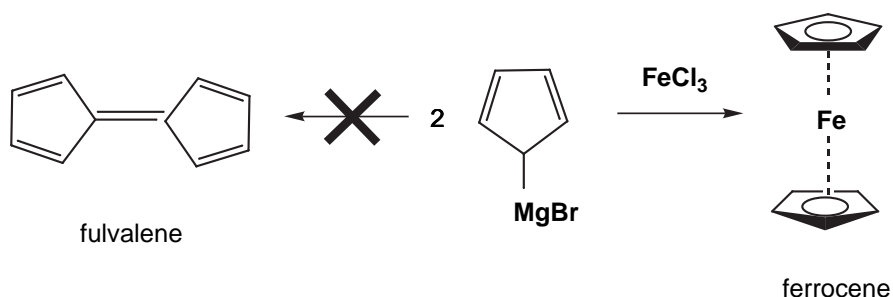


Figure 4.12 The structure of ferrocene.

An Fe atom caught between two cyclopentadiene rings. Literally a sandwich structure.

Exercise

4.1 Structures of inorganic compounds; the VSEPR theory

Suggest the structures of the following inorganic compounds.

- (a) SeF_6 (b) N_2O (c) ClO^- (d) CF_3Cl (C is the center)

Answer

- (a) octahedron (b) linear (c) linear (d) tetrahedron

4.2 Isomers of substituted benzenes

The molecular formula of a compound containing one benzene ring is C_8H_{10} . Draw the structural formulas of all possible isomers for this compound.

Answer

A C_8H_{10} compound containing one benzene ring is either ethylbenzene $C_6H_5C_2H_5$ or xylene $C_6H_4(CH_3)_2$. The latter compound has three positional isomers *i.e.*, *o*-, *m*- and *p*-xylene.

4.3 Geometrical isomers

Both fumaric acid and maleic acid have the rational formula $HOOCCH=CHCOOH$ and constitute a pair of geometric isomers. Upon heating at $150^\circ C$, maleic acid loses one mole of H_2O to give maleic anhydride while fumaric acid does not change to maleic anhydride until it is heated up to $300^\circ C$. Using this data, explain the structure of the two compounds.

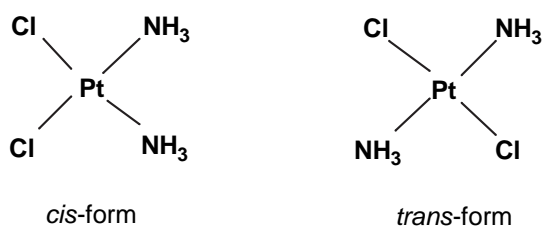
Answer

The answer is given in the text (p.xx).

4.4 The structures of platinum complex

Diamminedichloroplatinum $[PtCl_2(NH_3)_2]$ has a planar square structure. Guess the structure of possible isomers.

Two isomers, *cis*- and *trans*-form, are possible. The planar square structure is due to dsp^2 hybridization. The *cis* isomer is a famous anticancer drug.



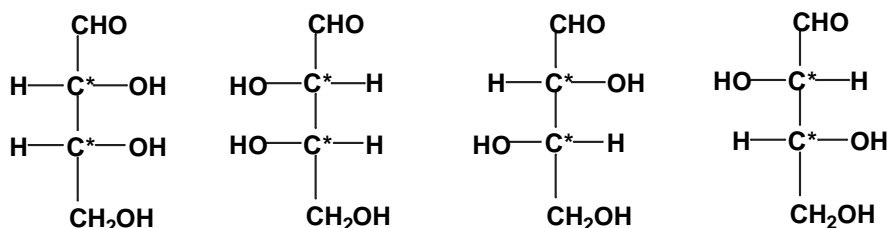
4.5 Stereoisomerism of sugars

This compound having four carbon atoms, $\text{HOCH}_2\text{CHOHCHOHCHO}$, is a sugar with simplicity comparable to glyceraldehydes.

- (a) How many asymmetric carbon atoms does this molecule have?
 (b) Draw the structural formulas for all the stereoisomers of this sugar in the manner shown in Fig. 4.5.

Answer

- (a) Two. In the structure below, the asymmetric carbon atoms are indicated by *.
 (b) Two pairs of enantiomers are clearly indicated.



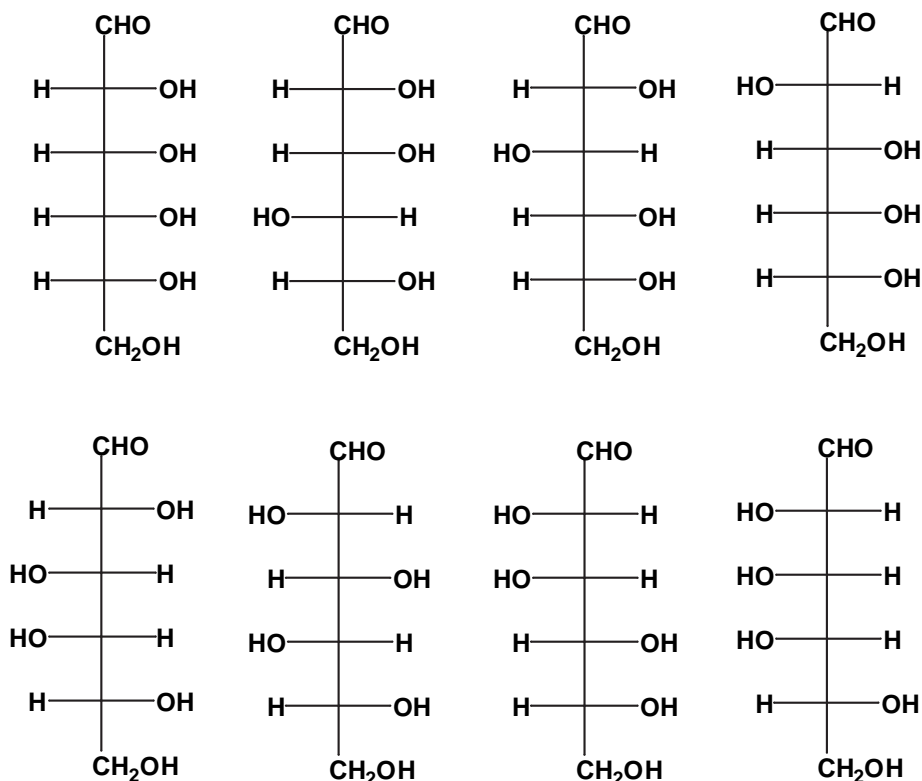
4.6 Stereoisomerism of glucose

Glucose, $\text{HOCH}_2(\text{CHOH})_4\text{CHO}$, has six carbon atoms and is one of the most abundant naturally occurring compounds

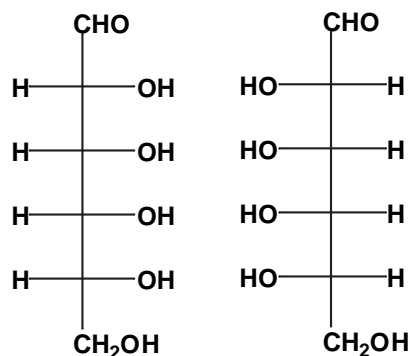
- (a) How many asymmetric carbon atoms does this molecule have?
 (b) Draw the structural formulas for all stereoisomers of this sugar in the manner shown in Fig. 4.5.

Answer

- (a) Four. In the structure below, the asymmetric carbon atoms are indicated by *.
 (b) The number of stereoisomers is $2^4 = 16$. The structures of eight isomers are shown.



For each of them, you can write the enantiomeric pairs as shown below.

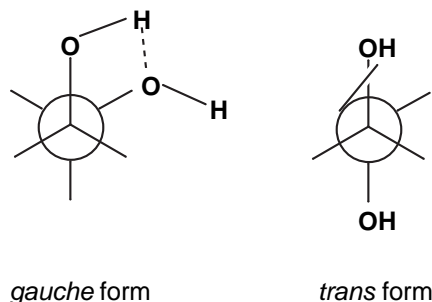


4.7 Conformational analysis of conformers

In the case of 1,2-dichloroethane, the *trans* form is more stable than the *gauche* form. On the other hand, in the case of ethylene glycol (1,2-ethanediol; widely used as an antifreezing fluid) the *gauche* form is more stable than the *trans* form although the molecular structure is very similar to 1,2-dichloroethane. Explain.

Answer

In the *gauche* form of ethylene glycol an intramolecular hydrogen bonding takes place which stabilizes the structure. Such bonding is absent in the *trans* form.



4.8 The bonding in diborane

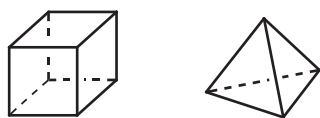
Explain the bonding in diborane.

Answer

See the text (p. xx).

Coffee Break---Compounds having interesting structures

There are a good number of organic compounds which have interesting and peculiar structures. A wonderful example is cubane C_8H_8 which is literally cubic. Although many techniques have been tried, the tetrahedral molecule, tetrahedrane C_4H_4 , has not yet been synthesized. The $\angle C-C-C$ bond angle is too different from the normal tetrahedral angle, and probably that is the reason why the synthesis has not yet been achieved.



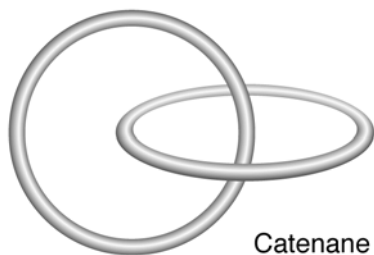
cubane

tetrahedrane

For simplicity's sake, labels for the atom and C-H bonds are omitted

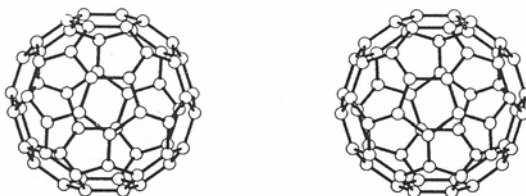
Another series of compounds with an interesting and even more peculiar structure are the catenanes, ring molecules that are puzzling. How can these two rings intertwine though there is no

chemical bond between them! How could chemists prepare such a compound? Indeed, this is one of the most brilliant achievements that modern synthetic organic chemistry has achieved.



Catenane
(schematic drawing)

Since its discovery at the end of the 20th century, fullerene C_{60} has attracted the attention of both theoretical and practical chemists. The ball is made of a combination of hexagon and pentagon, and indeed is very similar to a soccer ball. It is interesting to note that the possible existence of fullerene was predicted, long before its discovery, by the Japanese chemist Eiji Osawa.



fullerene(stereoview)