Forming molecules from their isolated constituent atoms can most simply, as a first
approximation, be thought of as "building up" of bonds between pairs of atoms. Thus, each
individual atom maintains roughly its atomic identity except that its valence electrons (and
sometimes, to a lesser extent, its core electrons) interact with "neighboring" atoms and their
valence electrons to form what we will call bonds. The major force that governs the "bonding
process" is the electromagnetic force, that is, the force that is present when we have interacting
electrical charges (either "stationary" = electrostatic (Coulombic) force or "moving" =
electromagnetic force). For most explanations, which will be qualitative rather than rigorously
quantitative, we will consider only "simple" electrostatic or Coulombic effects.

Thus, we envision bonding as a balance between the repulsions among "like particles" (valence
electrons with each other and nuclei with each other) and the attractions among "unlike particles"
(valance electrons with nuclei and vice versa). The relative strength of these two opposing
effects is a function of the distance between the constituent atoms and their relative location, i.e.,
it is "geometry dependent". For a given molecule, at a certain temperature and pressure, there is
a lowest energy geometry or "structure", in which the constituent atoms have "maximized" the
attractive and "minimized" the repulsive interactions. Such a geometry is energetically so
"favorable" to the isolated, unbonded, separated atoms, that the molecule "stays together" and is
thus "formed". The relative distance between each pair of atoms in the molecule are termed bond
lengths. Although these bond lengths are often difficult to obtain to high precision and often
difficult to obtain to high precision and often must be "measured" indirectly, they can be
determined accurately enough so that they may serve as a useful working concept. Also, the
relative location of the atoms can be obtained within the limits imposed by quantum theory -
we can thus speak of a molecule's geometry.

It would be useful if we could develop a model (necessarily qualitative, for our purposes) that
allows us to predict, based on the electronic structure of the isolated atoms, the experimental
structure of the molecule they conspire to form. First, we develop rules, based upon experimental
evidence, that allow us to see how the valence electrons arrange themselves to form the observed
bonding arrangements or bond types. These rules will allow us to classify bonds as either: ionic,
polar covalent, or (pure) covalent. The classification parameter is the electronegativity difference
(Δ) between the atoms participating in the bond. So,

Let \( x_A \) = electronegativity of atom A and \( x_B \) = electronegativity of atom B.

\[
\Delta x = \left| x_A - x_B \right| = \text{magnitude of the electronegativity difference between atoms A and B.}
\]

If \( \Delta x = 0 \) (Exactly) \( \Rightarrow \) AB bond is purely covalent (or non-polar) i.e., the electrons in the
bond are "equally shared".

If \( 0 < \Delta x \leq 1.7 \) \( \Rightarrow \) AB bond is polar covalent, i.e., the electrons are "polarized" toward
the more electronegative atom of the bond. However, both atoms
still have at least some "ownership" of the electrons in the bond.

If \( \Delta x > 1.7 \) \( \Rightarrow \) AB bond is ionic, i.e., the electrons in the bond are "totally owned"
by the more electronegative atom and "totally lost" by the less
electronegative atom of the bond. Thus, the less electronegative
atom becomes a positively charged ion (cation) and the more
electronegative atom becomes a negatively charged ion (anion).
Binary ionic compounds are "relatively simple to depict", since they consist of their separated isolated ions with the electrons suitably distributed so as to give the "properly charged" ionic species according to the periodic table. Such ionic structures show only valence electrons, i.e., those electrons that are "outside" of the noble gas core. It is felt that these electrons play the most significant role in molecule formation, when a chemical process occurs. The GUIDING PRINCIPLE is:

**In the formation of a stable molecule the constituent atoms will strive to achieve a Noble Gas Core configuration.**

That is to say, the valence electrons will "arrange themselves" among the atoms so that each atom has a "filled" valence shell, either by gaining the necessary electrons to fill the partially empty shell or by losing electrons to "return" to the "filled core". Structures that follow this guiding principle are often termed LEWIS STRUCTURES, after the chemist who pioneered this principle.

We will concentrate the major portion of our efforts on purely covalent and polar covalent molecules. These molecules may be as small as two atoms or may be fairly complex polyatomic molecules or even polyatomic ions. **Covalent** (pure and polar) species are said to consist of electron-pair bonds, i.e., bonds in which the electrons are at least "partially owned" by both atoms. Such covalent species comprise a large portion of interesting and/or common chemical compounds. In fact, "most" molecules or polyatomic ions are polar covalent species.

The Guiding Principle above is still valid in covalent molecules, except that now electrons in bonds are shared by both atoms in each atom's attempt to achieve a noble gas configuration. Thus, even though the sharing may be in fact unequal, as in a polar covalent bond; it is equal enough to satisfy both atoms, as they strive to attain "filled shells". So, when deciding "how to distribute" electrons in the molecule we must see how many valence electrons each atom is intrinsically imbued with when isolated and what it "has to do" (gain or lose electrons) to achieve a noble gas like valence shell in the "easiest manner".

We will only consider MAIN GROUP compounds, that is, compounds consisting of MAIN GROUP ATOMS (Groups 1A, 2A, 3A, 4A, 5A, 6A, 7A, and 8A). Hydrogen (H), in Group 1A, needs only one (1) electron more than what it has, in order to achieve a noble gas configuration (like Helium (He)). Thus, we say that Hydrogen, in covalent species, only needs to form one two-electron or single bond - in order to achieve its desired configuration. Thus, Hydrogen is said to obey a Duet Rule. Except for a "few exceptions", which will consist of atoms they "obey" an OCTET RULE: that is:

**Most Main Group Atoms will form compounds such that the constituent atoms create an s^2 p^6 valence shell configuration. This is because the Noble gases below Helium, have this valence shell configuration. Striving for a Noble gas configuration is the Guiding Principle.**

Thus, we say that atoms need eight (8) electrons around them, either "shared in bonds" with neighboring atoms or as a compromise between sharing in bonds and "keeping some electrons" for itself, i.e., not in bonds. Electrons that an atom does not have to "share in bonds" are termed unshared or non-bonded or lone electrons. Since these lone electrons commonly occur in groups of two, they are sometimes called lone pair electrons.

Unfortunately, the above guiding principle alone, does not tell us which atom is connected to which other atom, in other words, which atoms are next to which. Even more importantly, how are the atoms oriented spatially - what is the geometry of the molecule? The guiding principle (Octet and Duet Rules) just tell us where the electrons "go" after the atoms are arranged in their proper connection sequence. Once we know the connection sequence, however, the above rules will tell us the kinds of bonds form. They are:
Single bond  ⇒  2 electrons
Double bond  ⇒  4 electrons
Triple bond  ⇒  6 electrons

The above rules also tell us where the lone pair electrons "go". However, once we have drawn such Lewis structures, there are other principles which will allow us to predict the geometry of the molecule, based on the arrangement of the lone pair electrons relative to the electrons in bonds. This is the subject of another hand-out. These rules are termed the VSEPR RULES - more about that "later"!

For now, we summarize the procedure for drawing Lewis structures, which is, of course, based on our guiding principle (Octet and Duet rules, for instance):

1. Know the order of connection of the atoms.
2. Count the total number of valence electrons, i.e., add together the number of valence electrons of the constituent atoms. These electrons are "common to the molecule". If the species is an anion, add the additional electrons to the previous total. For example, \( \text{SO}_4^{2-} \) has 2 more electrons than the 30 valence electrons arising from the constituent atoms. Thus, \( \text{SO}_4^{2-} \) has 32 total valence electrons to arrange. If the species is an cation, add the subtract the necessary electrons from the previous total number of valence electrons. For example, \( \text{NH}_4^+ \) has 1 less electron than the 9 valence electrons arising from the constituent atoms. Thus, \( \text{NH}_4^+ \) has 8 total valence electrons to arrange.
3. Obey the octet or duet rule, as necessary, on each atom. Sometimes, double or triple bonds will be necessary to achieve this. Remember, lone pair electrons count for only the atom with which they are associated; whereas electrons in bonds contribute to the octet rule "count" for both atoms in the bond.

As mentioned previously, there are some exceptions to some of these rules and there is no substitute for practice.

**Lewis Structures, Resonance, Isomers, & Formal Charge**

This model of chemical bonding - according to G. N. Lewis (sometimes termed the Lewis-Langmuir model in earlier texts) - predated the development of quantum mechanics and was published by Lewis (Journal of the American Chemical Society - April 1916) at about the time of the Bohr model of the hydrogenic atom. [In fact, Lewis makes a comment in his article about the ludicrous hypothesis by Bohr in which he (Bohr) states that an electrostatically attracted circulating charged particle may exist in a stable orbit!!]

Previously we summarized the rationale behind Lewis structures. In this section, we will show - by way of several examples - how to systematically draw Lewis structures and also show how more than one Lewis structure, i.e., arrangement of electrons, may arise for a given arrangement of atoms. **When there exists more than one electron distribution (electron arrangement) for a given arrangement of atoms in a molecular species, these alternative electron distributions are termed resonance structures.** Then, we will introduce the concept of **formal charge (FC)** and exemplify how to use it to select the best Lewis structure from among a selection of valid resonance structures.
If there is more than one possible arrangement of atoms (geometry) for a molecular species of specific molecular formula, the possible atomic arrangements (geometries) corresponding to this singular molecular formula are termed (structural) isomers.

Your text lists the rules for drawing Lewis structures. Our version is summarized below. After we discuss and exemplify octet (duet) structures, we will discuss and exemplify exceptions to octet (duet) structures. These exceptions fall into the two categories: "expanded octets" (so-called - 10 electron and 12 electron species) as well as "electron-deficient" species (so-called - 4-electron (quartet) and 6-electron (sextet) species).

**RULES FOR WRITING LEWIS STRUCTURES**

1. **Determine the arrangement of atoms, i.e., the connectivity.**
   If more than one arrangement is possible - i.e., if more than one isomer is possible, follow these rules for each isomer - unless a specific isomer is given in the problem.

2. **Count the total number of valence electrons present.**
   - For a neutral (no net charge) molecule, the total number of valence electrons is just the sum of the valences of the individual atoms (determined by each atom's location in the periodic table).
   - For an anion (a net negative charge), the total number of valence electrons is once again the sum of the valence electrons of the individual atoms plus the number of additional electrons that give rise to the net negative charge.
   - For a cation (a net positive charge), the total number of valence electrons is once again the sum of the valence electrons of the individual atoms minus the number of electrons missing that give rise to the net positive charge.

3. **Evaluate each of the bonding regions as either covalent or ionic.**
   - If $\Delta x$ (defined above) is $> 1.7$ for a particular bonding region, the bond is said to be ionic.
   - If $\Delta x$ (defined above) is $\leq 1.7$ but $> 0$, the bond is considered polar covalent. If $\Delta x$ is exactly zero (0), the bond is considered (pure) covalent or non-polar (covalent). In either case, i.e., for polar or for non-polar covalent the Lewis rules are identical.

4. For an ionic structure, the atom with the greater electronegativity gains control of all of the electrons needed to form an octet - forming an anion that is isoelectronic with the closest noble gas of greater atomic number. The atom with the smaller electronegativity loses control of its electrons and becomes a cation - returning to its "noble gas core".
5. For a **covalent structure**, first try **single covalent bonds** between each pair of atoms and add lone pairs as needed to fulfill the octet (8) rule (or duet (2) rule for H) for each atom in the species.

6. For the **covalent structure**, then compare the total number of electrons used in the "single-bonded" structure with the total number of valence electrons available.

   (6a) If the totals match, you have a viable Lewis structure.

   (6b) **If not** - and if you **used too many electrons** in the "single-bonded" structure (the usual situation - why?) - **you must create more bonds**, i.e., **share more of the valence electrons**. So, determine how many "extra electrons" were used. This number - divided by two (2) - informs you of how many additional bonds must be added to the "single-bonded" structure. Add these additional bonds to the "single-bonded" structure - removing and rearranging lone pairs as needed to give the required octets (duets) - as necessary. If there is more than one way to achieve this "multiple bond" assignment that is consistent with the Lewis rules, write down each viable alternative. These are termed **resonance structures**.

   (6c) If more than one resonance structure is possible, assign formal charge (defined below) to each atom in each resonance structure and attempt to decide - via FORMAL CHARGE considerations - which - if any of the structures are better (best). If all of the structures are "equal" based upon formal charge assignments, then the structure of the molecule is a (resonance) hybrid - which can only be adequately explained using quantum mechanics!

As mentioned in the Lewis rules above, if there is more than one Lewis structure possible for a given arrangement of atoms, the concept of FORMAL CHARGE may help us decide if there is a "best" structure. For now, we give the definition of formal charge and how to calculate the formal charge (FC) on each atom for each Lewis structure that we draw. Later - by way of an example, we will show how to use formal charge assignments to decide on a "best" resonance structure.
The definition of formal charge (FC) on an atom "X" in a particular Lewis structure is:

\[ FC_X = (\text{valence of } X) - (\# \text{ bonds to } X + \# \text{ non-bonded } e^-'s \text{ around } X) \]

Formal charge assigned to an atom in a given Lewis structure is a parameter which "compares" the electronic environment of the atom in the Lewis structure to the electronic environment of the neutral isolated atom (i.e., its valence). So, if the atom has not deviated from its isolated electronic environment (valence) - but yet achieved the "noble gas stability" of a Lewis octet (duet), then this atom in the given Lewis structure has zero (0) formal charge. Prove this for yourself via the above formula. Such an atom has not "strained" its electronic environment relative to its valence, and yet has achieved "noble gas stability". Thus, zero formal charge indicates this "optimum" situation. So, zero formal charge or - more generally - minimum formal charge (i.e., minimum formal charge build-up or minimum "strain") is an important guiding principle when judging between several possible Lewis structures for a molecule or ion. The formal charge "rules" are summarized below. Consult your text for more details. As mentioned previously, a later example will show us how to use formal charge to make decisions.

One important result of formal charge assignment is that the SUM OF the FORMAL CHARGES ON ALL ATOMS IN A SPECIES MUST ADD UP TO THE NET CHARGE OF THE SPECIES, i.e,

- For a NEUTRAL MOLECULE ⇒ SUM OF FC's = 0 (no net charge).
- For an IONIC SPECIES ⇒ SUM OF FC's = (net - or net + charge).

[For example: For \( \text{NH}_4^+ \) the sum of FC's must = +1, while
For \( \text{PO}_4^{3-} \) the sum of FC's must = -3.]

Now we will list several examples - with little additional comment - except as necessary. Verify for yourself that the above steps have been followed.
• **Example # 1** : \[ \text{H}_2\text{O (water)} \], O is the central atom.
• Total of \(2(1) + 6 = 8\) total valence electrons.
• Each O–H bond is **polar covalent**.
• This is easy, since H can only form single bonds (duet rule).
  This leaves two (2) lone pairs of electrons around oxygen.
• The FC on oxygen and on each H is zero (0).

\[
\text{H} \quad \bigl\| \quad \text{O} \quad \bigl\| \quad \text{H}
\]

• **Example # 2** : \[ \text{NH}_4^+ \text{(ammonium cation)} \], N is the central atom.
• Total of \(5 + 4(1) - 1 = 8\) total valence electrons.
• Each N–H bond is **polar covalent**.
• This is easy, since H can only form single bonds (duet rule).
  This leaves no lone pair of electrons on nitrogen.
• The FC on nitrogen is +1 and each H has zero (0) FC.

\[
\begin{array}{c}
\text{H} \\
\text{H} \\
\text{N} \\
\text{H}
\end{array} + 
\]

• **Example # 3** : \[ \text{O}_2 \text{(molecular oxygen)} \]
• Total of \(2(6) = 12\) total valence electrons.
• The O–O bond is **pure covalent, i.e., non-polar**.
• Putting in all single bonds and lone pairs we have the following.

\[
\text{O} \quad \bigl\| \quad \text{O}
\]

\[
\text{Total number of electrons used} = 14 \\
\text{Total number of valence electrons} = 12 \\
\therefore \text{Number of excess electrons} = 2 \\
\Rightarrow 2/2 \Rightarrow \text{create 1 new bond}
\]
• Thus, we have a double-bonded structure, with each oxygen atom having a formal charge of zero (0). Convince yourself of this.

\[
\text{O} = \text{O}
\]
Example # 4: CN\(^-\) cyanide anion

- Total of 4 + 5 + 1 = 10 total valence electrons.
- The C–N bond is polar covalent.
- Putting in all single bonds and lone pairs we have the following.

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\[
\text{Total number of electrons used } = 14 \\
\text{Total number of valence electrons } = 10 \\
\therefore \text{ Number of excess electrons } = 4
\Rightarrow 4/2 \Rightarrow \text{create 2 new bonds}
\]

Thus, we have a triple-bonded structure, where the nitrogen atom has a formal charge of zero (0) and the carbon atom has a formal charge of –1! Convince yourself of this. Now nitrogen is the more electronegative atom - so - according to formal charge protocol, the nitrogen atom should have the –1 formal charge! But, any rearrangement of electrons to achieve this (prove for yourself) would destroy the Lewis octets. Octets prevail.

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Example # 5: Li\(_2\)O (lithium oxide), O is the central atom

- Total of 2(1) + 6 = 8 total valence electrons.
- Each Li–O bond is ionic! Since O is more electronegative than Li, O takes the single valence electron from each Li atom and achieves its octet by forming a –2 anion that is isoelectronic with the noble gas Ne. Each Li loses its single valence electron and thus each Li is isoelectronic with the noble gas He.
- The FC (and net charge) on oxygen is –2 and each Li has a +1 FC (and net charge).

\[
\text{Li}^{+1} \quad \left[ \begin{array}{c} \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \end{array} \right]^{-2} \quad \text{Li}^{+1}
\]

There are no covalent bonds present. This is an ionic compound!
Example # 6: $\text{O}_3$ (ozone), the O's connected in a row (OOO)

- Total of $3(6) = 18$ total valence electrons.
- Each O–O bond is pure covalent, i.e., non-polar.
- We proceed as in the last example. Putting in all single bonds and lone pairs we have the following.

\[ \text{O} = \text{O} = \text{O} \]

Total number of electrons used = 20
Total number of valence electrons = 18
\[ \therefore \text{Number of excess electrons} = 2 \]
\[ \Rightarrow 2/2 \Rightarrow \text{create 1 new bond} \]

- Convince yourself that there are two (2) structures that will fulfill the above constraint - without changing the relative position of any of the atoms. Thus, these structures are properly termed resonance structures. They are numbered I and II below. Also, convince yourself that the formal charge assignments (listed above each atom in each structure) are correct.

\[ \text{O} = \text{O} = \text{O} \quad \text{I} \quad \quad \text{O} = \text{O} = \text{O} \quad \text{II} \]

Both structures are equally good.

- Notice that neither I nor II has zero formal charge on all atoms. Also, notice that each structure is equally good/bad. But this is the best that we can do with a linear arrangement of atoms in order to fulfill the octet rule. Quantum mechanics would claim that Lewis theory fails here and that the "true" structure is a hybrid - not able to be specified by a single Lewis structure. This hybrid would be a linear arrangement of three oxygen atoms with neither double nor single bonds present. The equal resonance structures "tell" us that we have a structure with two equivalent O–O bonds that are "mid-way" between double and single bonds, i.e., a $\frac{1}{2}$ bond or bond order of 1.5!!

- Quantum mechanics would further say that the pair of electrons forming the "double" bond are actually delocalized over the entire molecule.
The resultant structure is sometimes depicted in the "non-Lewis" form, by showing the "half-bond" as a dashed line (---) "spread out" over both double bond sites.

\[
\text{O} \equiv \text{O} \equiv \text{O}
\]

Each O-O bond is thus predicted to be mid-way between a double and a single bond. A bond order of 1.5. A "delocalized structure" according to quantum mechanics!

We might predict that \(\text{O}_3(\text{g})\) should be an unstable molecule. Relative to \(\text{O}_2(\text{g})\) - for example - it is indeed!!

Note also that a triangular arrangement of oxygen atoms would give an octet structure with zero formal charge on each oxygen atom.

\[
\begin{align*}
\cdot & \quad \cdot \\
\cdot & \quad \cdot \\
\cdot & \quad \cdot \\
\end{align*}
\]

Even though this patches things up, the experimental structure of \(\text{O}_3\) is not triangular and the bonding between each pair of oxygen atoms is indeed found to be the same and in fact mid-way between single and double, i.e., two equivalent \(1 \frac{1}{2}\) bonds!

Experimental results rule! Formal charge arguments must sometimes be taken with a "grain of salt"!

**Example # 7** Let's consider the possible resonance structures of the cyanate anion (OCN\(^-\)) (i.e., C in the middle)

The Lewis structures - including resonance - are listed below. Fill in the missing details for yourself. This is crucial!

There are \(6 + 4 + 5 + 1 = 16\) valence electrons present. O–C and C–N bonds are (polar) covalent. The three (3) resonance structures are shown below and are numbered I, II, and III for reference.
• The formal charge (FC) is shown above each atom in each resonance structure.

Note that the sum of formal charges (FC) in each structure (I, II, & III) is −1.

Unlike the ozone example previously, this is the first time that all of the resonance structures do not have the same formal charge distribution on all atoms. How do we decide if there is a "best" structure? Here are the "rules"

• **Formal Charge "Rules" for picking a "Best" structure**

The following guidelines - based upon formal charge considerations - for discerning between "good" and "bad" Lewis resonance structures - should prove helpful.

1. **Formal charge build-up should be as low as possible, i.e., minimized.**
   This means that if a species is a neutral molecule, one should strive - if possible - for Lewis resonance structures where there is zero (0) formal charge on each and every atom. If this is not possible - due to the arrangement of atoms - or due to a net charge on the molecule (anion or cation), then "minimize" is still the rule. In other words, achieve as low a build-up of formal charge as possible on any one atom (+1 or −1 is better than +2 or −2, for example) and try to achieve as many "zeros" of formal charge as possible that is consistent with the net charge of the species. Any resonance structure that has the above qualities is considered the "most stable" or "preferred" structure (formal charge-wise). Note that if the net charge on a species is more than ±1, i.e., ±2, ±3, etc., "spreading out the burden" usually is the best approach. Thus, the ideal formal charge distribution for a polyatomic anion with net charge −2 is to have two (2) atoms with a −1 formal charge and the remainder of the atoms with 0 formal charge. This is usually better than the full −2 on one atom and zeros everywhere else. The key is "spread out the burden".

2. If formal charge build-up is unavoidable and has already been minimized, resonance structures with negative formal charge on the most electronegative atom (and/or positive formal charge on the least electronegative atom) are "most stable" or "preferrable" (formal charge-wise).
• Note: when deciding between isomers of a given molecule (i.e., between different atom arrangements), an isomer whose formal charge profile adheres most closely to items 1 and 2 above is usually the "preferred" or "most stable" isomer (formal charge-wise).

• Thus, by use of formal charge, one can often decide between the best arrangement of atoms (best isomer) and the best arrangement of electrons (best resonance structure) for the best isomer. This is an important skill which must be mastered and will be used over and over again in your study of chemistry - especially organic chemistry. Be sure not to confuse isomers with resonance structures! This is crucial!

Back to our example of the cyanate anion:

\[
\begin{bmatrix}
0 & 0 & -1 \\
\Omega & C & N
\end{bmatrix}^– 
\rightarrow 
\begin{bmatrix}
-1 & 0 & 0 \\
\Omega & C & N
\end{bmatrix}^– 
\rightarrow 
\begin{bmatrix}
+1 & 0 & -2 \\
\Omega & C & N
\end{bmatrix}^–
\]

The "best" structure, based on formal charge arguments, is II. Since the molecule has net charge (i.e., a −1 anion here), it is not possible to have a structure with zero (0) formal charge on every atom. The best compromise here is to have as low a build-up of formal charge as possible (−1, here) on one atom and zero (0) on all others. This minimizes the build-up of formal charge and yet yields the correct sum of formal charges. Since there must be a build-up of - at best - a −1 formal charge on one particular atom, it is best to have this negative formal charge on the most electronegative atom. According to the periodic trend in electronegativity, O is the most electronegative of the three (i.e., electronegativity of O > N > C). Think this all through carefully for yourself. Structure II achieves this result - thus it is the "best" structure. Neither III nor I are very good in comparison. In I, the minimum build-up of formal charge (−1, here) is on N - not the most electronegative atom. In III, there is greater formal charge build-up than either in I or in II. In addition, in III, there is positive formal charge on the most electronegative atom present - oxygen (O). Thus, III is the worst of all - by formal charge arguments.

\[
\begin{array}{c}
\text{III} \\
\text{worst}
\end{array} < 
\begin{array}{c}
\text{I} \\
\text{better}
\end{array} < 
\begin{array}{c}
\text{II} \\
\text{best}
\end{array}
\]

for the \(\text{OCN}^–\) anion!

It is clear from the three (3) structures II is the overall best resonance structure of \(\text{OCN}^–\) - based on formal charge considerations. In other words, structure II of the \(\text{OCN}^–\) anion has the minimum build-up of formal charge (−1, here) consistent with the net charge (−1, here) also, the required minimum negative formal charge is on the most electronegative of the 3 atoms present - oxygen (O).
So, structure II is considered the structure of cyanate anion (i.e., the resonance structure with a triple bond between C and N and a single bond between C and O. The other resonance structures are minor (or negligible) resonance contributors.

\[
\begin{array}{ccc}
-1 & 0 & 0 \\
\text{O} & \equiv & \text{C} \equiv \text{N} \\
\text{II}
\end{array}
\]

Note - It appears that atoms of low electronegativity (relatively) are better suited to be "central" atoms and not terminal atoms - based on formal charge considerations.

Finally, we list some "bonding patterns" for atom "X" which result in zero (0) formal charge on X - depending on the location of atom "X" in the periodic table. Specifically, we will consider the cases where atom "X" is - in turn - a Main Group (Column) element in Group 4A, 5A, 6A, and 7A, respectively. Verify this table for yourself.

- **Column 4A** [X could be C, Si, Ge, ...]  \( FC_X = 4 - (4 + 0) = 0 \)  
  (4 bonds and 0 lone pairs of electrons)
  
  \[
  \text{X} \\
  \text{X} \\
  \text{X} \]

- **Column 5A** [X could be N, P, As, ...]  \( FC_X = 5 - (3 + 1(2)) = 0 \)  
  (3 bonds and 1 lone pair of electrons)
  
  \[
  \text{X} \\
  \text{X} \\
  \text{X} \]

- **Column 6A** [X could be O, S, Se, ...]  \( FC_X = 6 - (2 + 2(2)) = 0 \)  
  (2 bonds and 2 lone pairs of electrons)
  
  \[
  \text{X} \\
  \text{X} \\
  \text{X} \]

- **Column 7A** [X could be F, Cl, Br, ...]  \( FC_X = 7 - (1 + 3(2)) = 0 \)  
  (1 bond and 3 lone pairs of electrons)
  
  \[
  \text{X} \\
  \text{X} \\
  \text{X} \]
Exceptions to the Lewis octet (duet) rule

- **Expanded Octets** (10 electrons or 12 electrons around an atom)

  As your text explains, some atoms can exceed an octet, i.e., have more than eight electrons surrounding them (bonding electrons plus lone pair electrons) when forming chemical bonds in a molecule. Such an atom is said to have an expanded octet. We will consider only the cases where the octet is "expanded" to either 10 or to 12 electrons around the atom. First, we must discuss the reason why an atom can have more than eight electrons surrounding it (i.e., more than eight electrons in its valence shell).

  Remember the origin of the octet (duet) rule. The idea was that an element will gain or lose or share electrons in a molecule so that its localized electronic environment in the molecule allows its valence shell to become isoelectronic with a noble gas. Thus, if the valence shell of the atom becomes isoelectronic with a noble gas, the atom will be chemically "satisfied" ("inert") locally. So, a first row atom, i.e., H, must achieve an electron configuration of $1s^2 = [\text{He}]$ - hence, the duet (2) rule for H. A second row element, i.e., Li, Be, B, C, N, O, F, - in order to become isoelectronic with a noble gas - has two choices. The atom can lose all of its valence electrons from the $n = 2$ shell - which is what happens to a metal in an ionic bond - and become isoelectronic with He. Or, the atom can fill its valence shell (i.e., achieve a valence shell electron configuration of $2s^2 2p^6$) and become isoelectronic with Ne. This latter situation - a filled $n = 2$ shell - gives rise to the octet (8) rule.

  For third row elements (and beyond) in the periodic table, the shell of highest principal quantum number ($n \geq 3$) can (at least) have an s-subshell, a p-subshell, and a d-subshell. To be specific, let's consider a third row element. A third row element has an outermost (valence) shell that can maximally accommodate 2 (for 3s), plus 6 (for 3p), plus 10 (for 3d) electrons. So, a filled shell can definitely accommodate more than eight electrons. Even though, in the case of isolated third row atoms, the 3d subshell remains empty until electrons at least begin occupying the 4s subshell, the 3d subshell is still close enough in energy to the 3s and 3p subshells to make it energetically accessible for bonding. Even though the maximum number of electrons that can fill the $n = 3$ shell is 18 (i.e., $2 + 6 + 10$), for common molecules forming from atoms in the Main Group (Groups 1A through 8A), 10 or 12 electrons is usually the maximum. Remember, when we start "packing" electrons around an atom - even if some of them are shared in bonds - the electron-electron repulsions begin to increase greatly. This is a destabilizing effect. Thus, the increased stabilization of chemical bond formation - due to an expanded octet - must be "weighed" energetically against the increased destabilizing repulsive effect of locally "packing" electrons around an atom. Hence, an expanded octet of 10 or 12 electrons is usually the limit.
How do we know whether or not to expand an octet on an atom? The first criterion - as discussed above - is that the atom must be in the third row of the periodic table or beyond (i.e., have available valence subshells beyond s and p). Second - in order to minimize the destabilizing electron-electron repulsions, the atom should be surrounded by as many atoms as possible. This will allow the stabilizing attractive interactions of the surrounding positive nuclei to partially "cancel" the effect of the electron-electron repulsions. Hence, the candidate atom for an expanded octet should be a central or interior atom in the molecule. Third, there should be some other contributing factor - such as good formal charge. Some examples should help clarify this. Your text also does several examples. You should work through those also.

• **Example # 8**: $\text{PO}_4^{-3} \text{ phosphate anion}$, P is the central atom
  - Total of $5 + 4(6) + 3 = 32$ total valence electrons.
  - The P–O bond is polar covalent.
  - Putting in all single bonds and lone pairs we have the following.
  - The formal charges (FC) that are different from zero (0) are listed.

  ![Lewis structure of PO₄⁻³](image)

  - Total number of electrons used = 32
  - Total number of valence electrons = 32
  - \[ \therefore \text{Number of excess electrons} = \text{none} \]
  - \[ \Rightarrow \text{valid Lewis octet structure} \]

  Note that the sum of formal charges (FC) is $-3$.

Since the molecule has a net charge (i.e., a $-3$ anion here), it is not possible to have a structure with zero (0) formal charge on every atom. The best compromise here is to have as low a build-up of formal charge as possible such that the sum of formal charges is still $-3$. The simplest way to do this - while minimizing the formal charge build-up on any one atom - is to have three (3) atoms with a $-1$ formal charge, and the remaining atoms (each) with a zero (0) formal charge. Since oxygen (O) is more electronegative than phosphorus (P), we might suppose that a $-1$ formal charge on three of the four oxygen atoms and a zero formal charge on the remaining oxygen atom...
- and also on the phosphorus atom - is the best course. Reference to the table of bonding patterns leading to zero formal charge (page 13), reveals that if oxygen is involved in a double bond with two pairs of lone pair electrons, it will have zero formal charge. Thus, if we "relocate" one of the non-bonding electron pairs on one of the oxygen atoms into a P–O bond, we will create a double bond between that oxygen and phosphorus and the doubly-bonded oxygen will have zero formal charge. However, even though oxygen still maintains an octet, phosphorus has now expanded its octet to 10 electrons! But, this is the ideal situation! Consider the three criteria listed above:
  • The atom is in the third row of the periodic table - or beyond.
    Phosphorus is in row 3 (i.e., \([\text{Ne}]3s^2 3p^3\), thus, a 3d subshell is available).
  • The atom is a central or internal atom. P is the central atom here.
  • Better formal charges result. Let's check this out.

We note that there are four (4) ways of creating a P–O double bond, i.e., four (4) oxygen atoms that can form a double bond with phosphorus. Hence, there are four (4) equivalent resonance structures - with identical formal charge assignments. The four ten-electron resonance structures - with formal charge assignments - are listed below. Check them for yourself.

Note that this is the best that we can do. There are three atoms (O) - each with the minimum amount of negative formal charge (i.e., $-1$) to yield the requisite net charge of −3. Also, the most electronegative atom (O) has the negative formal charge. Thus, the four resonance structures above are equivalent and as a group represent the preferred structure of \(\text{PO}_4^{3-}\). Note that the octet structure listed earlier is a minor (negligible) contributor. How then do we describe the "structure" of \(\text{PO}_4^{3-}\)?
Quantum mechanics would tell us that the "true" structure of $\text{PO}_4^{3-}$ is a (resonance) hybrid of the four structures just listed. The "true" structure of the phosphate anion is a single structure not representable by the typical Lewis picture - hence the four listed structures. The "true" structure is one in which there are four equivalent phosphorus-oxygen bonds, where each bond is a single bond plus one-quarter of a double bond, i.e.,

- $\text{P-O Bond Order} = 1 + \frac{1 \text{ bond delocalized over}}{4 \text{ bonding regions or sites}} = 1 + \frac{1}{4} = 1 \frac{1}{4}$

We might depict the structure in the non-Lewis form:

```
\[ \text{P} = \text{O} , \quad \text{O} \quad \text{O} \quad \text{O} \quad \text{O} \quad -3 \]
```

Four equivalent P-O bonds each with Bond Order B.O. = 1 1/4

Thus, fractional bond order (B.O.) results when there is more than one resonance structure that represents (due to formal charge assignment) an equally optimum alternative to the structure of the molecule. According to quantum mechanics, the single structure cannot be represented by a single Lewis structure, because part of the bonding picture arises from delocalization of electron density over all of the bonding regions (sites).

12 electron expanded octets:

There are species in which the octet may be expanded to 12 electrons around a suitable atom. A common example is $\text{SO}_4^{2-}$ anion. Work through it on your own and then check with your text. It is worked out as an example in your text.
• **Electron Deficient Species**

(4 electrons (*quartet*) or 6 electrons (*sextet*) around an atom - other than hydrogen)

As your text explains, some atoms - other than hydrogen - can have less than an octet of electrons when forming molecules. Atoms in this category tend to be Main Group elements that have fewer than four valence electrons ("metals") and that enter into polar covalent bonds - rather than into ionic bonds. Remember, if a metal atom enters into a bond with a non-metal atom such that $\Delta x \equiv |x_A - x_B| > 1.7$, an ionic bond will result where the metal atom will lose its valence electrons and the non-metal atom will gain these "lost" valence electrons so that both metal cation and non-metal anion achieve a valence shell electron configuration that is isoelectronic with the appropriate noble gas. However, if a metal atom enters into a bond with a non-metal atom such that $\Delta x \equiv |x_A - x_B| \leq 1.7$, a polar covalent or non-polar covalent bond will result. The most notable examples of this latter situation are the (polar) covalent compounds of beryllium (Be) and of Boron (B). We will consider them now.

• **(Polar) Covalent Beryllium (Be) compounds**

Let's consider $\text{BeCl}_2$ (beryllium dichloride).

**Example # 10**: $\text{BeCl}_2$, Be is the central atom

- Total of $2 + 2(7) = 16$ total valence electrons.
- The Be–Cl bond is *polar covalent*.
  
  $\Delta x \equiv |x_{\text{Cl}} - x_{\text{Be}}| = |3.0 - 1.5| = 1.5$

- We will try a single-bonded molecule with two (2) Be–Cl single bonds - leaving Be "electron-deficient" with only four (4) electrons surrounding it (as in the BeH$_2$ example above).

![4-electron structure](image)

Note that the FC on Be and on each Cl is zero (0). The above structure is what is observed experimentally.
• **Exercise**: Consider the possible octet structure of BeCl₂. The resonance structures and corresponding formal charge assignments are listed. Prove that the three listed octet structures are minor (negligible) resonance contributors compared to the four-electron (quartet) structure listed previously.

\[
\begin{align*}
\text{Cl} & \equiv \text{Be} \equiv \text{Cl} \\
\text{Cl} & \equiv \text{Be} \equiv \text{Cl} \\
\text{Cl} & \equiv \text{Be} \equiv \text{Cl}
\end{align*}
\]

Note - "poor" formal charge is **not** the reason for the quartet structure over the octet structures - merely rationalization after the fact!

• **(Polar) Covalent Boron (B) compounds**

There are several examples of "electron-deficient" six-electron boron (B) compounds. Actually, the chemistry and compounds of boron (B) are even more exotic than what we are revealing here! We will consider only BCl₃ (boron trichloride) here.

• **Example # 11**: BCl₃ , B is the central atom
  • Total of 3 + 3(7) = **24 total valence electrons**.
  • The B–Cl bond is **polar covalent**.
    \[ \Delta x \equiv |x_{\text{Cl}} - x_B| = |3.0 - 2.0| = 1.0 \]
  • We will try a single-bonded molecule with three (3) B–Cl single bonds - leaving B "electron-deficient" with only six (6) electrons surrounding it (as in the BH₃ example above).

\[
\begin{align*}
\text{Cl} & \equiv \text{B} \equiv \text{Cl} \\
\text{Cl} & \equiv \text{B} \equiv \text{Cl} \\
\text{Cl} & \equiv \text{B} \equiv \text{Cl}
\end{align*}
\]

Note that the **FC on B and on each Cl is zero (0)**. The above structure is what is observed experimentally.
Consider the possible octet structure of BCl₃. The resonance structures and corresponding formal charge assignments are listed. Prove that the three listed octet structures are minor (negligible) resonance contributors compared to the six-electron (sextet) structure listed previously.

\[
\begin{align*}
\text{Octet structures} \\
\begin{array}{c}
\text{Cl} \quad \text{B} \quad \text{Cl} \\
\quad \text{Cl} \\
\quad \text{Cl} \\
\quad \text{Cl} \\
\quad \text{Cl} \\
\quad \text{Cl} \\
\quad \text{Cl} \\
\quad \text{Cl} \\
\end{array}
\end{align*}
\]

Note - "poor" formal charge is not the reason for the quartet structure over the octet structures - merely rationalization after the fact!

So, now that you know how to draw the Lewis structure for a molecular or ionic molecular species, is there a way to determine the three-dimensional arrangement of the atoms, i.e., the molecule’s geometry? There is! The simplest - but yet very powerful - model is the Valence Shell Electron Pair Repulsion Model aka VSEPR model for short. The rules for applying this model to a "best" Lewis structure are detailed in your text and summarized in the next section. Please refer to your text in addition to the summary that follows.
The VSEPR (Valence-Shell-Electron-Pair-Repulsion) method provides a simple, reasonably accurate means of predicting molecular shapes. Sidgewick and Powell developed this method in 1940 and Gillespie continued the work more recently. The VSEPR method used the number of pairs of valence electrons around the central atom to predict the molecular geometry - ideally. This geometry is not the one observed - if some of these lone pairs (or non-bonded electrons) are not involved in bonds. Each lone pair "pushes" the bonds that it "repels" closer together, such that the interactions between lone pairs (L.P.) and electrons in bonds (Bonding Pairs = B.P.) follow the trend:

- L.P. vs L.P. > L.P. vs B.P. > B.P. vs B.P.

To apply the VSEPR method to molecules with double or triple bonds, one initially counts all bonds (single, double, triple) as equal concentrations of electronic charge - and predict the molecular geometry based on this assumption. Then, we modify our initial prediction by "realizing" that these "extra" electrons in the multiple bond(s) will "squash" the "other" (non-multiple or less-multiple) bonds "closer" together - thus, reducing these "other" bond angles further. For example, molecule ethene has the structure:

\[
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{H}
\end{array}
\begin{array}{c}
\text{C} \\
\text{H} \\
\text{H}
\end{array}
\quad \text{H–C–H bond angle = 117°}
\]

One considers each carbon to be surrounded by three (3) concentrations of electronic charge. Then, as VSEPR predicts (and we will see), the molecule will be planar and the H–C–H bond should be 120°. (As we will see, this geometry derives from sp² hybridization on each Carbon atom in the molecule.) Now, taking into account that there are more electrons between the carbon atoms than there are between the carbon and hydrogen atoms, we predict that each H–C–H bond angle will be less than 120°. The observed H–C–H bond angle is 117° (see above).

Thus, to determine the molecular (observed) geometry of a molecule, using the VSEPR approach, we follow the following recipe.

1. **Draw** the Lewis structure and **count** the total number of concentrations of electronic charge around the CENTRAL ATOM. This number, termed the Steric Number (S.N.), is given by:

   \[
   \text{S.N.} = \left( \# \text{ of Atoms bonded to the Central Atom} \right) + \left( \# \text{ of pairs of non-bonded or L.P. electrons around Central Atom} \right)
   \]

   Remember, multiple bonds count as one concentration of electronic charge when determining the steric number. Also, the octet rule, if ever disobeyed, should only be allowed to be disobeyed on the central atom - and then only if the central atom is "allowed" to do so.

2. **Check** the table to see the geometry of the "electron pairs" around the central atom. This is termed the **ideal geometry**.
3. Count the number of pairs of non-bonded (L.P.) electrons on the central atom and check the table to see how this changes the ideal geometry. This is termed the observed geometry.

4. Refine the bond angles due to multiple bonds, by realizing that the multiple bond "reduces" the "other" bond angles from the value predicted in step # 3. Remember the ethene example.

N.B. - Technically, the VSEPR rules do not apply to transition metal compounds, unless the metal has a filled, half-filled, or empty d-subshell. Below we summarize the results; along with the hybridization of the central atom. Refer to the text above for the definitions of the abbreviations used in the table below.

<table>
<thead>
<tr>
<th>S.N.</th>
<th>Ideal Geometry</th>
<th>L.P.</th>
<th>Observed Geometry</th>
<th>Example(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Linear sp (Later)</td>
<td>0</td>
<td>Linear</td>
<td>BeH₂, CO₂</td>
</tr>
<tr>
<td></td>
<td>X—A—X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>Trigonal planar (120° angles)</td>
<td>0</td>
<td>Trigonal planar</td>
<td>BF₃</td>
</tr>
<tr>
<td></td>
<td>sp² (Later)</td>
<td>1</td>
<td>Bent (&lt; 120°)</td>
<td>SO₂ (119.5°)</td>
</tr>
<tr>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>Tetrahedral (109°28' angles)</td>
<td>0</td>
<td>Tetrahedral</td>
<td>CH₄</td>
</tr>
<tr>
<td></td>
<td>sp³ (Later)</td>
<td>1</td>
<td>Trigonal Pyramidal (&lt; 109°)</td>
<td>NH₃ (107°)</td>
</tr>
<tr>
<td></td>
<td>X</td>
<td></td>
<td></td>
<td></td>
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Continued on Next Page
<table>
<thead>
<tr>
<th>S.N.</th>
<th>Ideal Geometry</th>
<th>Hybridization (Later)</th>
<th>L.P.</th>
<th>Observed Geometry</th>
<th>Example(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>Trigonal</td>
<td>dsp^3 (Later)</td>
<td>0</td>
<td>Trigonal Bipyramidal</td>
<td>PCl_5</td>
</tr>
<tr>
<td></td>
<td>Bipyramidal</td>
<td>dsp^3 (Later)</td>
<td>1</td>
<td>&quot;See-Saw&quot;</td>
<td>SF_4</td>
</tr>
<tr>
<td></td>
<td></td>
<td>dsp^3 (Later)</td>
<td>2</td>
<td>&quot;T-shape&quot;</td>
<td>ClF_3</td>
</tr>
<tr>
<td></td>
<td></td>
<td>dsp^3 (Later)</td>
<td>3</td>
<td>Linear</td>
<td>XeF_2</td>
</tr>
</tbody>
</table>

![Diagram of a trigonal bipyramidal geometry](image)

| 6    | Octahedral     | d^2sp^3 (Later)       | 0    | Octahedral        | SF_6       |
|      |                | d^2sp^3 (Later)       | 1    | Square Pyramidal  | IF_5       |
|      |                | d^2sp^3 (Later)       | 2    | Square Planar     | XeF_4      |

![Diagram of an octahedral geometry](image)
VSEPR & Dipole Moments:
Polar versus Non-Polar Molecules

When there is an electronegativity difference \( \Delta x = |x_A - x_B| \), between two atoms in a covalent bond, we have a polar covalent bond. Because of the "shift" in electron density toward the more electronegative atom; the atom of lower electronegativity has a fractional or partial positive charge \( \delta^+ \) and the atom of higher electronegativity has a fractional or partial negative charge \( \delta^- \). We say that each polar (covalent) bond \((A-B)\) has a BOND DIPOLE MOMENT \( (\mu_{\text{bond}}) \). This bond dipole moment is symbolized by an arrow \( (-|--->) \) directed toward the more electronegative atom; along the \((A-B)\) bond axis. Assuming that the electronegativity of atom \( B \) is greater than that of atom \( A \), i.e., \( x_B > x_A \), we have:

\[
\begin{align*}
A & \quad \delta^+ \\
\quad & \quad \delta^- \\
\quad & \quad B
\end{align*}
\]

Bond Dipole Moment if \( (x_B > x_A) \)

In general, the dipole moment \( (\mu) \) is non-zero when there is an overall separation of charge (i.e., an overall \( \delta^+ \) and \( \delta^- \)). Specifically, the magnitude of \( \mu \) is defined as the product of the charge that is separated \( (\delta) \) and the distance of separation \( (r) \):

\[ \mu = \text{dipole moment} = \delta r \]

In SI units, the unit of charge \( (\delta) \) is Coulombs, the unit of distance \( (r) \) is meters; hence the unit of dipole moment \( (\mu) \) is Coulombs meters. Commonly, dipole moments are expressed in the unit of Debyes \( (D) \). Specifically,

\[ 1 \text{ Debye} = 1 \text{ D} = 3.34 \times 10^{-30} \text{ Coulombs meters} \]

Dipole moments \( (\mu) \) are vector quantities, i.e., they have both magnitude and direction. We have already said that the dipole moment for a specific polar covalent bond \( (\mu_{\text{bond}}) \) points along the bond axis of that bond. However, even though a molecule has polar bonds (i.e., has several bond dipole moments); under a suitable geometrical arrangement of the polar bonds, the bond dipole moments \( (\mu_{\text{bond}})'s \) could add up to zero, i.e., "cancel". In such situations, we say that the NET DIPOLE MOMENT \( (\mu_{\text{net}}) \) is ZERO and the molecule is NON-POLAR (there is no net separation of charge). Otherwise, if \( \mu_{\text{net}} \) is NON-ZERO, the molecule is POLAR (there is a net separation of charge). Summarizing:

\[
\begin{align*}
\mu_{\text{net}} &= \text{vector sum of } \mu_{\text{bond}}'s = 0 \quad & \text{NON-POLAR MOLECULE} \\
\mu_{\text{net}} &= \text{vector sum of } \mu_{\text{bond}}'s \neq 0 \quad & \text{POLAR MOLECULE}
\end{align*}
\]

What we would like to be able to do (at least) is to be able to predict if a molecule is polar or if it is non-polar. Using the VSEPR rules and the corresponding predicted geometries, we can make a reasonable guess as to whether a molecule is polar or non-polar; based upon the arrangement of bonds and the cancellation (or non-cancellation)
of bond dipole moments. Following, is a table which lists geometrical arrangements of polar bonds which give rise to NON-POLAR MOLECULES ($\mu_{\text{net}} = 0$). Check these out carefully, for yourself, to make sure you agree. Before we list this table, we give the dipole moment of some "common" molecules.

<table>
<thead>
<tr>
<th>Molecule</th>
<th>Net Dipole Moment ($\mu_{\text{net}}$) in Debyes</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{H}_2$</td>
<td>0 D</td>
</tr>
<tr>
<td>$\text{H}_2\text{O}$</td>
<td>1.94 D</td>
</tr>
<tr>
<td>$\text{NH}_3$</td>
<td>1.46 D</td>
</tr>
<tr>
<td>$\text{CH}_4$ or $\text{CCl}_4$</td>
<td>0 D</td>
</tr>
<tr>
<td>$\text{CH}_3\text{Cl}$</td>
<td>1.86 D</td>
</tr>
<tr>
<td>$\text{CH}_2\text{Cl}_2$</td>
<td>1.60 D</td>
</tr>
<tr>
<td>$\text{CHCl}_3$</td>
<td>1.03 D</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Non-Polar Molecules (Molecular Geometries with $\mu_{\text{net}} = 0$)</th>
<th>Ideal geometry &amp; S.N.</th>
<th>Example(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{X}$$\text{A}$$\text{X}$</td>
<td>Linear S.N. = 2</td>
<td>BeH$_2$, CO$_2$, $\text{X}$$\text{C}$$\equiv$$\text{C}$$\text{X}$</td>
</tr>
<tr>
<td><img src="image" alt="Trigonal Planar" /></td>
<td>Trigonal Planar S.N. = 3</td>
<td>BF$_3$, SO$_3$</td>
</tr>
<tr>
<td>$\text{X}$$\text{A}$$\text{X}$</td>
<td>Tetrahedral S.N. = 4</td>
<td>CH$_4$, CCl$_4$</td>
</tr>
</tbody>
</table>

Continued on Next Page
<table>
<thead>
<tr>
<th>Non-Polar Molecules (Molecular Geometries)</th>
<th>Ideal geometry &amp; S.N.</th>
<th>Example(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trigonal Bipyramid S.N. = 5</td>
<td></td>
<td>PF$_5$ = &quot;I&quot;</td>
</tr>
<tr>
<td>&quot;I&quot; = AX$_5$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>or</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trigonal Bipyramid S.N. = 5</td>
<td></td>
<td>PF$_3$Cl$_2$ = &quot;II&quot;</td>
</tr>
<tr>
<td>&quot;II&quot; = AX$_3$Y$_2$</td>
<td>(X = F, Y = Cl)</td>
<td>XeF$_2$ = &quot;II&quot;</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(X = ••, Y = F)</td>
</tr>
<tr>
<td>Octahedral S.N. = 6</td>
<td></td>
<td>SF$_6$ = &quot;III&quot;</td>
</tr>
<tr>
<td>&quot;III&quot; = AX$_6$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>or</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Octahedral S.N. = 6</td>
<td></td>
<td>SF$_4$Cl$_2$ = &quot;IV&quot;</td>
</tr>
<tr>
<td>&quot;IV&quot; = AX$_4$Y$_2$</td>
<td>(X = F, Y = Cl)</td>
<td>XeF$_4$ = &quot;IV&quot;</td>
</tr>
<tr>
<td>or</td>
<td></td>
<td>(X = F, Y = ••)</td>
</tr>
<tr>
<td>Octahedral S.N. = 6</td>
<td></td>
<td>SF$_2$Cl$_2$Br$_2$ = &quot;V&quot;</td>
</tr>
<tr>
<td>&quot;V&quot; = AX$_2$Z$_2$Y$_2$</td>
<td>(X = F, Y = Br, Z = Cl)</td>
<td>XeF$_2$Cl$_2$ = &quot;V&quot;</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(X = F, Y = ••, Z = Cl)</td>
</tr>
</tbody>
</table>