A Convenient Approach for the Construction of Lewis Structures by Focusing on the Valence Requirements of Outer Atoms

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***Abstract*:** A convenient approach to obtain Lewis structures for compounds of the type YX_n involves first constructing a trial structure that satisfies the valence of the outer atoms (*e.g.* 1 bond for fluorine, 2 bonds for oxygen and 3 bonds for nitrogen) and placing the molecular charge (if any) on the central atom. The second step involves evaluating the electron count of the central atom, which can give rise to three possibilities: (i) if the central atom has an octet configuration, no change in the number of bonds is required, (ii) if the central atom (Y) exceeds the octet, a Y–X bond is relocated as a lone pair on X, which results in a formal positive charge on Y and a formal negative charge on X, and (iii) if the electron count on the central Y atom is less than an octet, a lone pair on the outer atom is relocated as a Y–X bond, which results in a formal negative charge on Y and a formal positive charge on X; these transformations modify the electron configuration around X such that it will adopt a correct Lewis structure. This approach differs considerably from other methods that require one to first calculate the total number of valence electrons. As such, the method described here, which focuses on using valence as a guiding chemical principle, is much less mathematically oriented and therefore less subject to errors from incorrect calculations.

Keywords: Lewis structures, formal charge, covalent bond, octet rule, general chemistry.

Introduction

Lewis structures[1-3] are simple representations of molecules that derive from (i) the use of "dots" to represent the valence electrons of atoms and (ii) the notion that a covalent bond between two atoms is a consequence of them sharing a pair of electrons. Despite their simplicity, however, these two-dimensional representations are of pivotal importance in chemistry because, in conjunction with the so-called octet rule,[2,4,5] they provide a means to evaluate the chemical reasonableness of a molecule. Furthermore, together with VSEPR theory, the Lewis structure allows one to predict the three-dimensional shape of a molecule.[6] In addition to providing rudimentary information concerned with the bonding and structure of a molecule, the Lewis structure representation of organic molecules provides an important component of describing reaction mechanisms in terms of well-established electron pushing formalisms,[7] an approach that has more recently been extended to inorganic chemistry.[8]

As a consequence of this utility of Lewis structures, it is not surprising that their construction features prominently in elementary chemistry courses, for which a variety of approaches have been introduced. In this regard, the method that the majority of textbooks employ for drawing the Lewis structure of a molecule, for which the connectivity is either known or assumed (with the least electronegative atom, except hydrogen, often assumed to be the central atom), is that the student first sums the total number of all valence electrons in the molecule; these electrons ("dots") are then assigned as either bond pairs or as lone pairs, with the intention of having each atom achieve an octet configuration (where possible).[9]

Depending upon the molecule under consideration, the above process can be mathematically intensive, although it has the apparent advantage of requiring little knowledge of chemistry.[9g] A problem with this method, however, is that the introduction of a simple mathematical error will cause confusion that will inherently result in an incorrect Lewis structure;[9a,10] unfortunately, this error can only be recognized by appealing to chemical insight (see the Supporting Information for examples of such problems). Since a degree of chemical understanding is ultimately required to evaluate the accuracy of a Lewis structure, it is rational to use such knowledge at the outset for their construction. Therefore, this article provides a less mathematically oriented approach for the construction of Lewis structures, with the extra benefit that formal charges (*i.e.* the charges remaining on the atoms when all bonds are broken homolytically) arise without the need for any additional computation. This approach complements other approaches that have been introduced for drawing Lewis structures that do not focus on computing the total number of valence electrons.[11]

Common Bonding Motifs

A critical component of the approach developed here is to ensure that a student fully understands the electronic impact on an atom upon the formation of a normal covalent bond. Such understanding may be obtained by considering the bonding in neutral XH_n compounds (X = C, N, O, F) and recognizing how many normal covalent bonds the atom X needs to form in order to attain an octet configuration (*i.e.* its common valence), which also corresponds to the value of 18 minus the Periodic Table group number.

Prior to discussing XH_n compounds, however, it is pertinent to consider first the Lewis structure for the simplest molecule, namely H_2, as illustrated in Figure 1. Two hydrogen atoms, each with a single electron, form a covalent bond by sharing the electrons such that each hydrogen has a duet configuration (*i.e.* that of helium). The pair of electrons in the bond is conventionally replaced with a line in the final Lewis structure. In the approach developed here, the electrons on two different atoms are represented as a "dot" and a "cross"[2] for clarity to indicate that they originate from two different atoms.

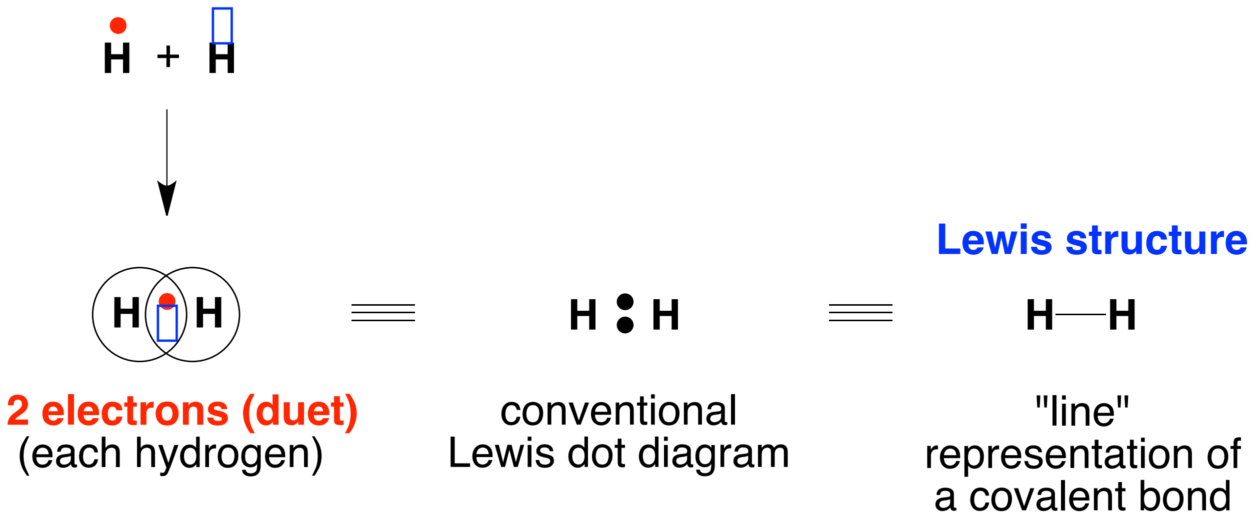

Figure 1. Construction of the Lewis structure for H_2. Each hydrogen atom has a single electron that is represented as a red dot and blue cross to indicate that they originate from different atoms. Sharing of these electrons results in the duet configuration for each hydrogen (bottom left) and the electrons are represented as black dots in the conventional Lewis dot diagram (bottom center), and as a line in the more commonly used Lewis structure representation (bottom right).

The procedure for constructing Lewis structures for XH_n molecules requires first identifying the number of valence electrons associated with X, which simply corresponds to its position in the Periodic Table, as summarized in Table 1. The second step is to determine the number of hydrogen atoms that need to be attached to X such that it achieves an octet configuration. As an illustration, consider the conceptual formation of CH_4 (Figure 2). The carbon atom possesses four valence electrons and the formation of a bond with hydrogen to generate CH increases the electron count of carbon by one. Specifically, the carbon atom is associated with a shared pair of electrons comprising the C–H bond and three nonbonding electrons (*i.e.* $2 + 3 = 5$). Since CH does not have an octet configuration, this process is conceptually repeated to obtain CH_4, at which point the carbon possesses an octet configuration and exhibits a valence of four (Table 1), with no remaining nonbonding electrons on carbon. Representing pairs of bonding electrons as lines, the conventional Lewis structure of

CH_4 thus has carbon with four lines attached to hydrogen atoms (Figure 2), with no lone pair electrons.

Table 1. Common valences of C, N, O and F as determined by their position in the Periodic Table.

	C	N	O	F
Periodic Table Group	14	15	16	17
Number of valence electrons (m)[a]	4	5	6	7
Common valence (n)[b]	4	3	2	1
XH_n formula[c]	CH_4	NH_3	H_2O	HF
Electron count of X in XH_n	8	8	8	8

(a) Note that the number of valence electrons corresponds to the last digit of the Periodic Table group.

(b) The valence of an atom is the number of electrons that it has used in bonding. Note that, for these elements, the common valence is equal to 18 minus the Periodic Table group number.

(c) Note that the molecular formula of the commonly encountered hydrogen compounds corresponds to the common valence.

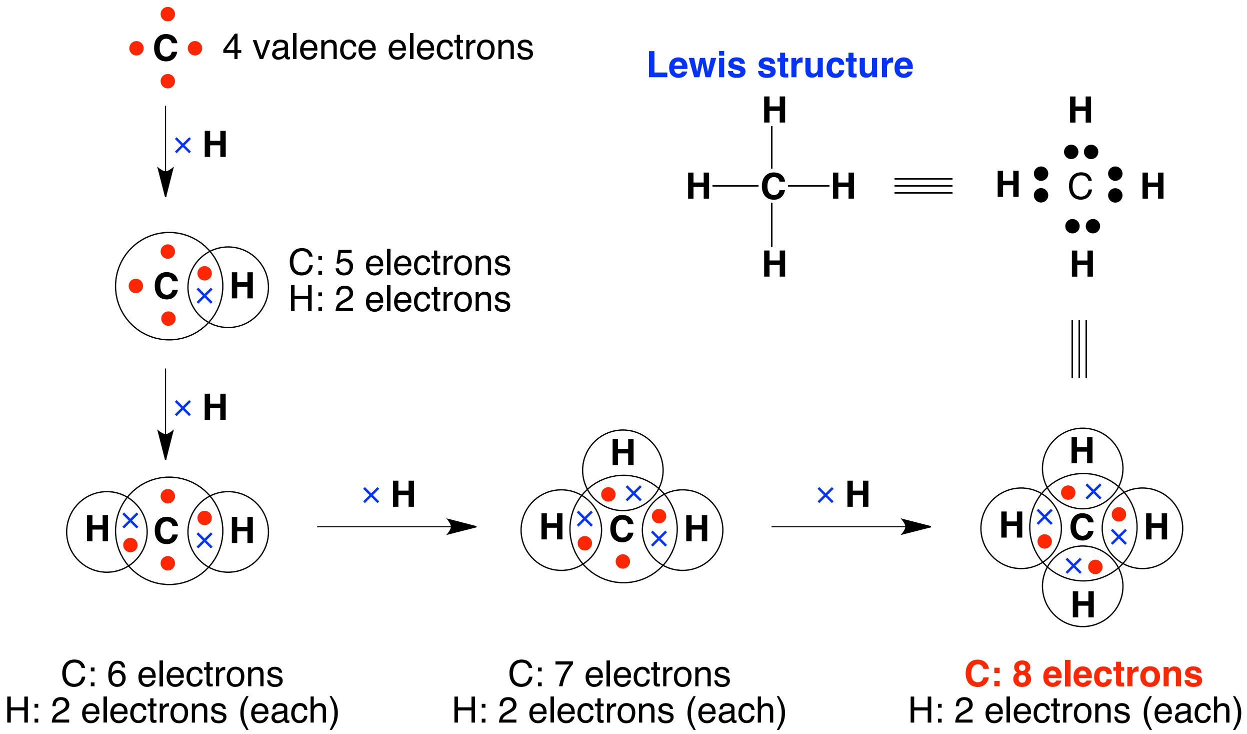

Figure 2. Construction of the Lewis structure for CH_4. The electrons originating from the carbon are represented as red dots while those from the hydrogen atoms are indicated by blue crosses, with the sole purpose of emphasizing the concept that a normal covalent bond is a shared pair of electrons in which each atom contributes one electron. The addition of each hydrogen to carbon (i) increases the overall electron count on carbon by one, (ii) decreases the number of nonbonding electrons on the carbon by one and (iii) increases the valence of carbon by one. The octet configuration is achieved when four hydrogen atoms have been added and carbon is tetravalent.

Performing the analogous procedure for nitrogen, which has five valence electrons (Table 1), indicates that an octet configuration is achieved upon addition of three hydrogen atoms to afford NH_3, such that nitrogen exhibits a valence of three (Figure 3).

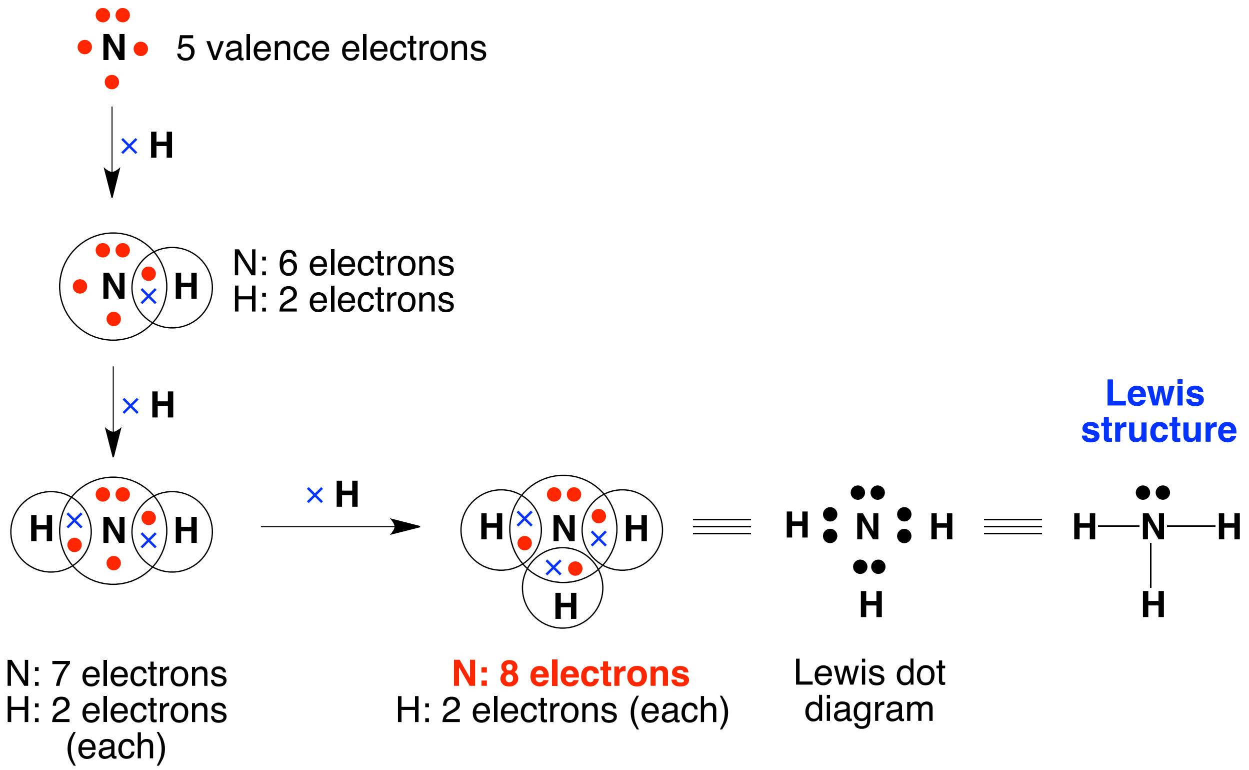

Figure 3. Construction of the Lewis structure for NH_3. The electrons originating from the nitrogen are represented as red dots while those from the hydrogen atoms are indicated by blue crosses, with the sole purpose of emphasizing the concept that a normal covalent bond is a shared pair of electrons in which each atom contributes one electron. The addition of each hydrogen to nitrogen (i) increases the overall electron count on nitrogen by one and (ii) decreases the number of nonbonding electrons on the nitrogen by one. The octet configuration is achieved when three hydrogen atoms have been added, with the result being that two nonbonding electrons (*i.e.* a lone pair) remain on nitrogen.

In contrast to CH_4, the nitrogen does not use all of its valence electrons in arriving at the octet configuration and so two nonbonding electrons, *i.e.* a lone pair, remain on the nitrogen atom. Similar considerations indicate that oxygen needs to bind two hydrogen atoms to achieve an octet configuration, while fluorine only binds a single hydrogen atom. Consequently, the oxygen and fluorine atoms have respectively two and three lone pairs in H_2O and HF (Figure 4). The molecular formulas of the neutral XH_n molecules thus correspond to the number of bonds that must be drawn to a neutral X atom in order for it to achieve an octet configuration and hence provide a very useful aide memoire for drawing Lewis structures. As would be expected, the same rationale applies to the heavier congeners. It is also worth noting that, while it is advantageous to achieve an octet configuration, it is not always possible. For example, since boron has only three valence electrons, it can only bind to three hydrogen atoms with the result that BH_3 possesses a sextet configuration. The sextet configuration confers high reactivity to BH_3 such that that it exists as a dimer under normal conditions, B_2H_6, with a bonding description that features 3-center-2-electron interactions, which is beyond the scope of this paper.[12]

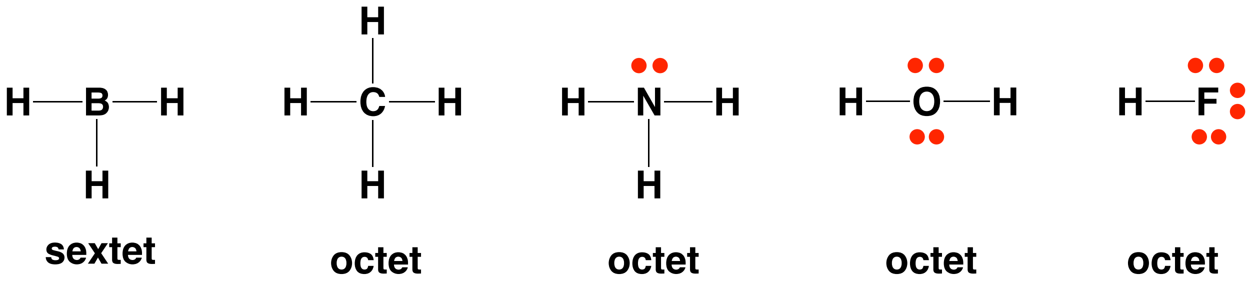

Figure 4. Comparison of the Lewis structures of XH_n. Note that in moving from carbon to fluorine fewer hydrogen atoms are required to achieve the octet configuration of X, such that the number of nonbonding electrons increases in this sequence. Boron possesses only three valence electrons and so can only bind three hydrogen atoms, such that the neutral hydride, BH_3, does not possess an octet.

The above stepwise construction of CH_4 and NH_3 makes it evident that the formation of every covalent bond to a neutral atom X results in (i) ***the electron count of the atom increasing by one*** and (ii) ***the number of nonbonding electrons decreasing by one***. Recognizing this relationship makes it clear to a student how many bonds an atom X needs to form in order to achieve an octet configuration, and also how many nonbonding electrons (*i.e.* twice the number of lone pairs) will remain on the atom after forming these bonds (Table 2).

Table 2. Important Considerations for Construction of Lewis Structures

Upon formation of a normal covalent bond to an atom: (1) the electron count increases by one (2) the number of nonbonding electrons decreases by one
Upon placing a formal positive charge on an atom: (1) the electron count decreases by one (2) the number of nonbonding electrons decreases by one
Upon placing a formal negative charge on an atom: (1) the electron count increases by one (2) the number of nonbonding electrons increases by one
Bonds and lone pairs associated with neutral atoms: carbon (4 bonds, 0 lone pairs) nitrogen (3 bonds, 1 lone pair) oxygen (2 bonds, 2 lone pairs) fluorine (1 bonds, 3 lone pairs)

It is important to emphasize that the above construction of the Lewis structures of CH_4, NH_3, H_2O and HF should be presented in a very detailed manner so that afterwards a student is able to (i) reproduce them in an efficient manner and (ii) clearly recognize how many bonds and lone pairs are associated with a neutral atom (Table 2). In particular, it is essential to recognize that each atom possesses a combined total of four bond and lone pairs that are distributed in such a manner that carbon forms four bonds, nitrogen forms three bonds, oxygen forms two bonds and fluorine forms one bond in these compounds (*i.e.* the common valences of these elements).

In addition to considering the number hydrogen atoms that are needed to coordinate to a neutral atom in order for it to achieve an octet configuration, it is instructive to consider charged variants and appeal to isoelectronic relationships. For example, a cationic nitrogen N^+ species is isoelectronic with carbon and so it also requires four bonds to achieve an octet, resulting in the ammonium ion, $[NH_4]^+$ (*cf.* CH_4). Correspondingly, an anionic boron B^- species is also isoelectronic with carbon and so likewise requires four bonds to achieve an octet, resulting in the tetrahydroborate ion, $[BH_4]^-$. With respect to oxygen, cationic O^+ is isoelectronic with N and so it forms $[H_3O]^+$ (*cf.* NH_3), while anionic O^- is isoelectronic with F and so forms $[HO]^-$ (*cf.* HF). While it is not essential to remember the compositions of these charged species in order to apply the approach described below, familiarity with these motifs (Figure 5) is useful because they appear so frequently in Lewis structure representations. Thus, albeit not necessary, knowledge that a neutral oxygen atom appears with two bonds, a cationic oxygen atom possesses three bonds, and an anionic oxygen possesses a single bond considerably facilitates the evaluation of a proposed Lewis structure.

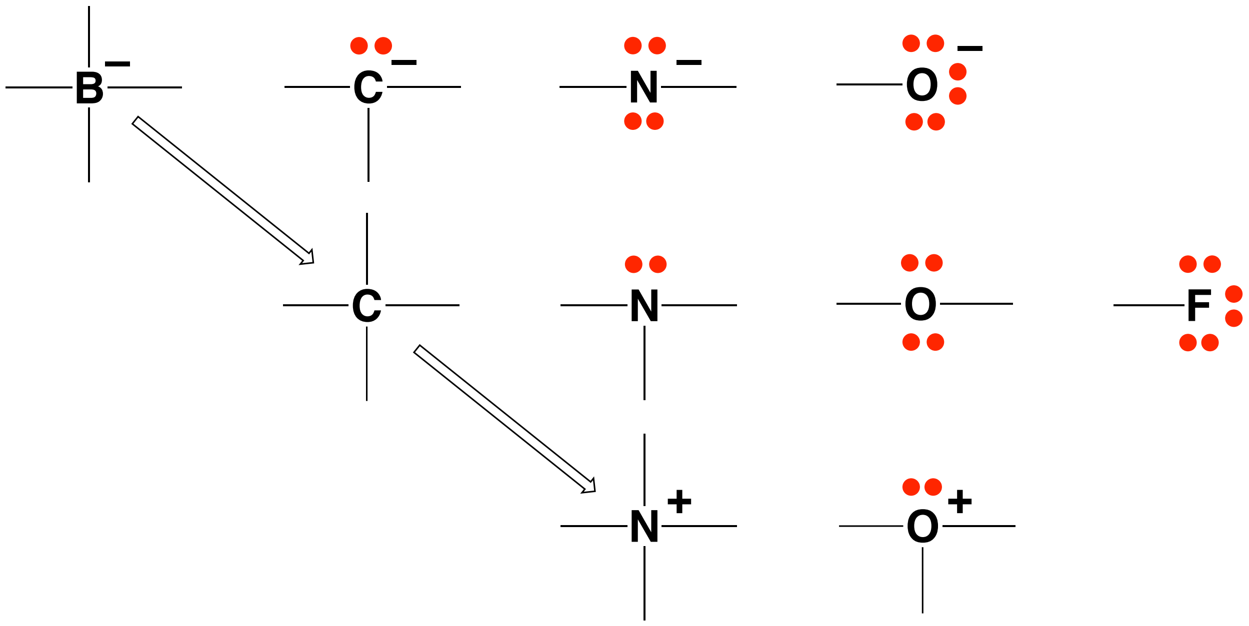

Figure 5. Commonly observed bonding motifs for B, C, N, O and F with octet configurations. Note that the formal charge is zero when the number of bonds is the same as the commonly observed valence as indicated by the composition of XH_n (center line) and that, in order to preserve the octet configuration, the formal charge increases as additional bonds are added for a given element (vertical relationship, *e.g.* OH^-, H_2O, and H_3O^+). In addition to the vertical relationship, note the diagonal relationship that relates isoelectronic species (*e.g.* $B^- \equiv C \equiv N^+$). Similar motifs apply to the heavier congeners of these elements.

Constructing Lewis Structures of YX_n Molecules By Using the Valence Requirements of Outer atoms

Equipped with the knowledge obtained by constructing the Lewis structures of CH_4, NH_3, H_2O and HF (Figure 4), Lewis structures for other molecules (for which the connectivity is either given or assumed) can be obtained by performing several simple steps.

1. Produce a trial structure by drawing bonds between the central atom (Y) and the outer atoms (X) that correspond to the valence requirements of the outer atoms as indicated by the number of bonds in XH_n (Figure 4). For example, this would involve

drawing two bonds to an oxygen atom (and its heavier congeners) and one bond to a fluorine atom (and its heavier congeners). Add lone pairs to the outer atoms that correspond to those in the neutral XH_n molecules such that they will have an octet configuration, recognizing that the sum of bond pairs and lone pairs is four (Figure 4). A distinct advantage of this approach is that it means that the outer atoms are ***necessarily drawn correctly with octets in the trial structure***, such that attention only needs to be given to the central atom; furthermore, the electron configurations of the outer atoms will also automatically be drawn correctly upon applying the transformations described below (if needed).

2. If the molecule is charged, place the charge on the central atom.

3. Evaluate the nature of the central atom with respect to the number of electrons that are associated with the valence shell, *i.e.* the electron count. Recognizing that each bond adds one electron, the electron count (EC) is simply the sum of the number of valence electrons on the neutral atom (m) and the number of bonds (b), after taking into account any charge that has been placed on the atom (Table 3). This approach for counting electrons, which is equivalent to simply adding the number of valence electrons on the central atom to the number of electrons provided by the outer atoms in bonding, is analogous to the neutral method for counting electrons in organotransition metal compounds within the context of the 18–electron rule.[13]

4a. If the electron count is eight, *i.e.* the central atom has an octet configuration, then the representation is valid and all that is necessary is to add lone pairs to the central atom (if necessary); see below #5 (Table 3).

Table 3. Procedure for determining the electron count and number of nonbonding electrons on an atom.

electron count (EC)	**number of nonbonding electrons (#NB)**
EC = $m + b - Q$	#NB = $m - b - Q$
m = number of valence electrons on central atom (Table 1) b = total number of bonds Q = charge on the atom	

4b. If the central atom (Y) exceeds the octet (*i.e.* appears hypervalent[14]), then it is necessary to move one or more pairs of Y–X bonding electrons (typically from a multiple bond but sometimes from a single bond) so that they become localized on outer X atoms (Figure 6); this procedure decreases the electron count of the atom from where they are moved, but does not change that of the atom for which they become a lone pair. Importantly, the transfer of electrons from a Y–X bond pair to an X lone pair results in the creation of a formal positive charge on Y and a formal negative charge on X (since an electron that originated on Y is now located on X).[11d] In some cases, this process may need to be repeated to achieve an octet configuration, at which point nonbonding electrons are assigned to the central atom. It must be emphasized that formal charges are not real charges, but are an important component of electron bookkeeping.[15] As such, a complete Lewis structure not only displays the bonds and nonbonding electrons (lone pairs), but also incorporates formal charges.

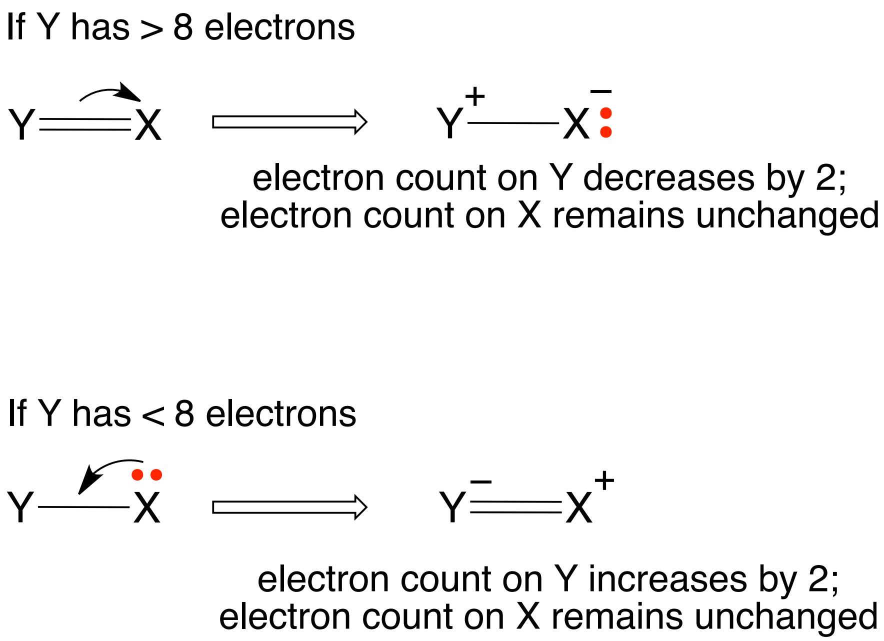

Figure 6. Creation of formal charges associated with decreasing (top) or increasing (bottom) the electron count of the central atom (Y).

4c. If the central atom Y has less than an octet configuration (*i.e.* appears hypovalent, which is not as common), then it is necessary to use a lone pair of electrons on X to form an additional Y–X bond, which is the opposite of step #4b. As such, this transfer of electrons from X to Y (*i.e.* a dative covalent bond)[16] results in the creation of a formal negative charge on Y and a formal positive charge on X (Figure 6); note that the electron count of the donor atom is not reduced when using a lone pair to form a bond because the electrons are shared by both atoms. It should be recognized that, in rare cases, it may not be possible to achieve an octet configuration, as exemplified by BH_3, $[CH_3]^+$ and molecules with odd numbers of electrons.

5. Once a Lewis structure with an octet configuration has been achieved, assign nonbonding electrons to the central atom by subtracting the number of bonds from the number of valence electrons on the neutral atom and adjusting for the charge (Table 3).

The advantage of this approach is that a trial structure can be arrived at immediately and, in the event that it is not the correct structure, then modifications can be made to adjust the structure in a well-defined rational manner using simple chemical principles. While some degree of mathematics is required (Table 3), it is better described as "counting". For example, determining the electron count of the central atom is simply performed in a visual sense by taking the number of valence electrons of the neutral atom and "counting up" one for each bond that is attached and adjusting for the charge if necessary. Note that this simple approach for obtaining the electron count does not require one to determine first whether there are any nonbonding electrons on the atom, which is necessary if it were to be determined by using the alternative expression [(2 × number of bonds) + number of nonbonding electrons].

Correspondingly, the number of nonbonding electrons is determined by "counting down", namely taking the number of valence electrons of the neutral atom and removing one for each bond that is attached and adjusting for the charge if needed.

As a simple illustration, consider NF_3 (Figure 7). Following step #1, a trial structure is produced by drawing a nitrogen atom attached *via* single bonds to three fluorine atoms, each of which has three lone pairs. Since the charge on the molecule is zero (step #2), the electron count of the nitrogen in step #3 is eight (Table 3), which is obtained by taking the five valence electrons on nitrogen and "counting up" one for each of the three bonds. Since it has an octet (step #4a), the next step is to determine the number of nonbonding electrons (step #5), which is obtained by starting with the five valence electrons on the nitrogen atom and "counting down" by one for each of the three bonds, thereby resulting in two nonbonding electrons, *i.e.* a single lone pair. Should one so desire, these calculations can be performed by applying the formulas listed in Table 3 and Figure 7, but they are more effectively performed by the "counting" procedure without the need to write anything down. Thus, while the total of 8 for the electron count could be determined by simply adding 5 and 3, the process of starting with 5 and then simply adding one for each bond counted minimizes mathematical errors. Likewise, while the number of nonbonding electrons could be determined by subtracting 3 from 5, the process of starting with 5 and then sequentially reducing the number for each bond present also minimizes mathematical errors.

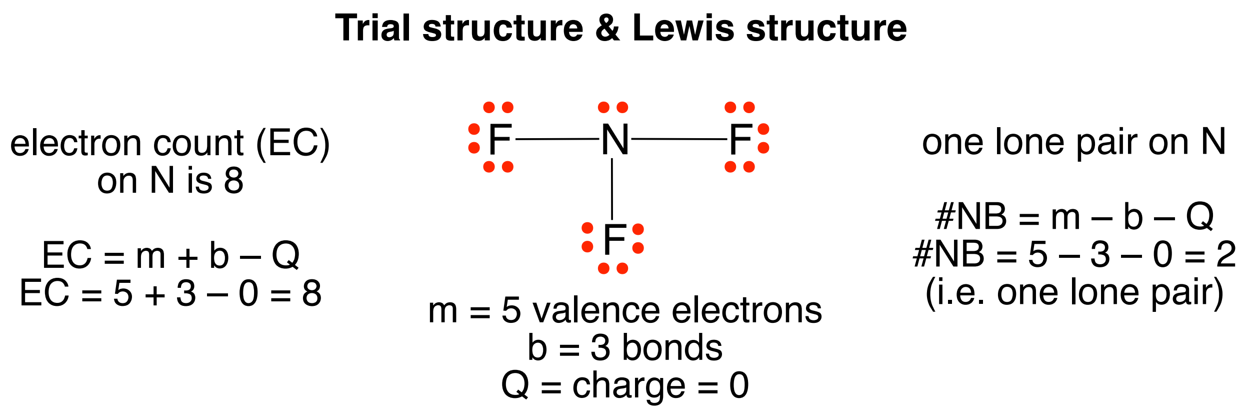

Figure 7. Trial structure for NF_3 obtained by drawing one bond between nitrogen and each of the three fluorine atoms. The nitrogen has an octet configuration and one lone pair and, in this case, the trial structure is the correct Lewis structure.

This procedure is chemically more appealing than one that simply sums the valence electrons of a nitrogen atom (5) and three fluorine atoms (3 × 7 = 21) and then requires the 26 electrons to be distributed in pairs in a manner that assigns 8 electrons to each atom. While this approach may be satisfactory for certain molecules, for others the approach has been described as requiring "trial and error", as illustrated by CO_2.[17] In contrast, the approach described here gives the correct Lewis structure for CO_2 at the first step (Figure 8). Thus, simply drawing double bonds between the carbon atom and the two outer oxygen atoms results in a carbon atom that has an octet configuration with no lone pairs and so is the correct Lewis structure.

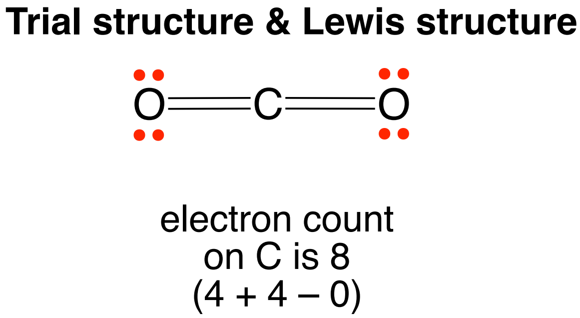

Figure 8. Trial structure for CO_2 obtained by drawing two bonds from oxygen to carbon, which has an octet configuration for carbon. In this case, the trial structure is the correct Lewis structure.

Ozone is structurally related to CO_2 and so the trial structure for O_3 involves drawing a central oxygen atom to two outer oxygen atoms with double bonds. However, the central oxygen atom in this structure has an electron count of ten such that it exceeds the octet configuration. The situation is, nevertheless, readily reconciled by moving one of the bonding pairs of electrons to an outer oxygen atom. Not only does this result in the central oxygen atom having an octet configuration, but it also results in it having a formal positive charge while the outer oxygen atom has a formal negative charge, which is the accepted Lewis structure for ozone. Note how the assignment of the formal charges arrives naturally and ***does not require any additional calculations***. As such, this is a considerable advantage over methods that require formal charges to be calculated *via* a separate procedure, which becomes increasingly laborious as the number of atoms in the molecule increases. In addition, it is pertinent to note that the oxygen atoms in this molecule have the three bonding motifs for oxygen that are shown in Figure 5. Thus, the oxygen atom with two bonds has no formal charge, the oxygen atom with three bonds has a positive formal charge, while the oxygen atom with a single bond has a negative formal charge.

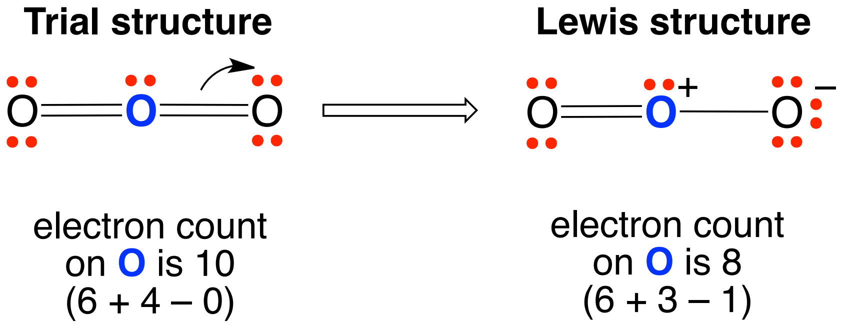

Figure 9. Trial structure for O_3 obtained by drawing two bonds from the outer oxygen atoms to the central oxygen atom (left). The presence of the single lone pair on the central oxygen atom in the trial structure is determined by "counting down" from 6 (the number of valence electrons on an oxygen atom) by one for each O–O bond. The central oxygen atom has a dectet configuration and moving a bond pair to an outer atom, thereby becoming a lone pair, results in an octet configuration for the central atom. Note how (i) the formal charges on the atoms appear automatically and require no further calculation and (ii) the three different motifs of the oxygen atoms in the Lewis structure correspond to those shown in **Figure 5**.

In addition to moving a bond pair to the right oxygen in the trial structure of Figure 9, it is also possible to move the bond pair to the left, thereby resulting in a resonance structure (Figure 10). The bonding in O_3 is thus a hybrid of these two structures with a formal covalent bond order (bo) of 1.5 between each pair of oxygen atoms.

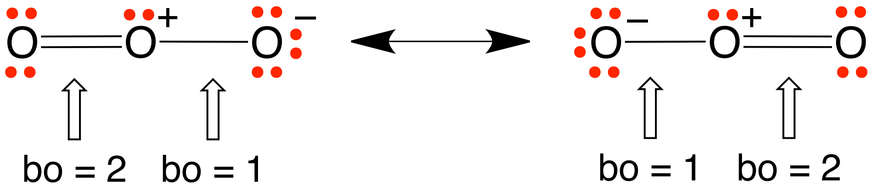

Figure 10. Resonance structures for O_3 (bo = covalent bond order).

A linear trinuclear neutral molecule that features nitrogen in the central position is N_2O. The trial structure for this molecule involves a triple bond between the central nitrogen atom and the outer nitrogen atom and a double bond between nitrogen and the oxygen atom (Figure 11). However, with this configuration, the central nitrogen atom has an electron count of ten such that it exceeds the octet configuration. As with O_3, the situation is reconciled by moving one of the bonding pair of electrons to an outer atom (either oxygen or nitrogen).

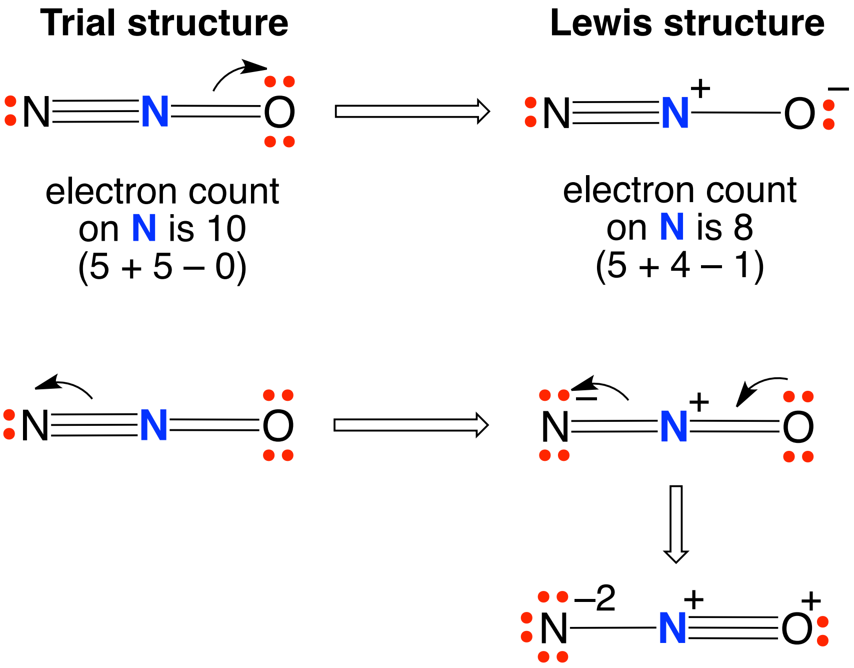

Figure 11. Trial structure for N_2O obtained by drawing three bonds from the outer nitrogen atom and two bonds from the oxygen atom (left). The central nitrogen atom has a dectet configuration, and moving a bond pair to an outer atom, thereby becoming a lone pair, results in an octet configuration (right). Note that the bond pair that is moved can be either an N–O bond (top) or an N–N bond (center). In addition, a third Lewis structure can also be drawn.

While this situation is very similar to that of ozone, it must be emphasized that the two resonance structures for N_2O are not degenerate and thus contribute differently to the overall description of the molecule (Figure 12). In addition to having Lewis structures with (i) an N≡N triple bond and (ii) an N=N double bond, it is also possible to have one with a single N–N bond by transferring another pair of N–N bonding electrons to a lone pair on the outer nitrogen atom (Figure 12). However, since this decreases the electron count of the central nitrogen by two units, it is necessary to compensate by transferring a lone pair of electrons from the oxygen atom to an N–O bonding pair, thereby resulting in a N≡O triple bond (Figure 11 and Figure 12).

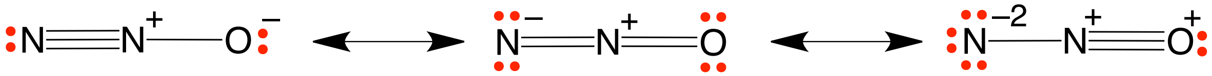

Figure 12. Resonance structures for N_2O. In contrast to O_3, the resonance structures are not degenerate and so do not have equal weight in describing the bonding.

An example of a cationic trinuclear molecule is provided by $[NO_2]^+$. In this case the trial structure is constructed by drawing double bonds between nitrogen and the two oxygen atoms, while the positive charge is placed on the central nitrogen atom (Figure 13). Consideration of the electron count of the nitrogen atom indicates that it has an octet configuration and thus the trial structure is also the Lewis structure. In addition, there are no nonbonding electrons on the nitrogen because, of the five electrons on a neutral nitrogen atom, four are used in forming bonds to the two oxygen atoms and one is removed as a consequence of the formal positive charge. It is also pertinent to note the similarity of the Lewis structure of $[NO_2]^+$ to that of CO_2 (Figure 8), which is a natural consequence of the fact that N^+ is isoelectronic with C.

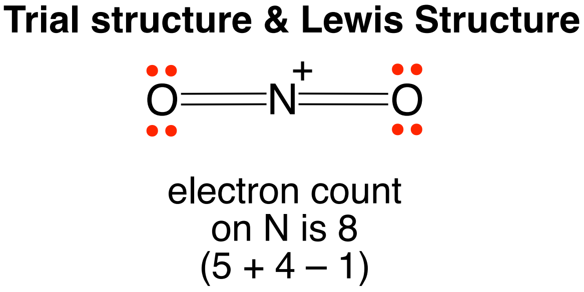

Figure 13. Trial structure for $[NO_2]^+$ obtained by drawing two bonds from oxygen to nitrogen and placing the positive charge on the nitrogen, thereby resulting in an octet configuration for nitrogen. In this case, the trial structure is the correct Lewis structure.

The trial structure for the anionic nitrite anion, $[NO_2]^-$, is drawn similarly to that for $[NO_2]^+$ except that the charge placed on the nitrogen is negative (Figure 14). The nitrogen atom of the trial structure thus has a dectet configuration that may be rectified by moving an N–O bonding pair to a lone pair on oxygen. As with the other examples, the negative formal charge on the oxygen is obtained without computation. It is also relevant to note the formal analogy between the bonding in $[NO_2]^-$ and O_3 (Figure 10) as a consequence of N^- being isoelectronic with O.

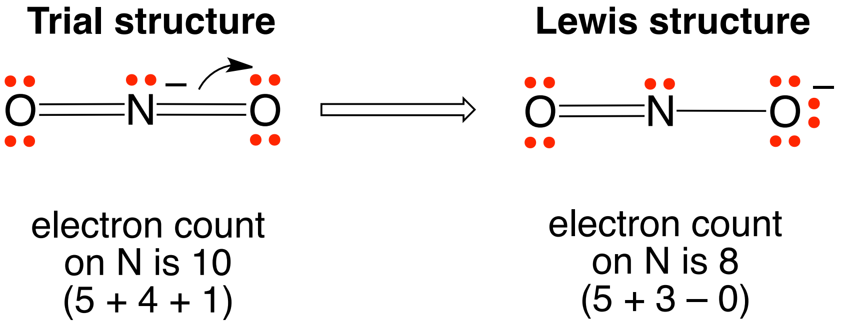

Figure 14. Trial structure for $[NO_2]^-$ obtained by drawing two bonds from the outer oxygen atoms to the central nitrogen atom and placing the negative charge on nitrogen (left). The nitrogen atom has a dectet configuration and moving a bond pair to a lone pair on the oxygen atom results in an octet configuration (right).

The Lewis structure of the nitrite anion displays a lone pair of electrons on nitrogen that in a formal sense may be used to bind an oxygen atom to afford the nitrate anion, $[NO_3]^-$. The trial structure of $[NO_3]^-$ is one in which the nitrogen atom is attached by double bonds to three oxygen atoms and the negative charge is localized on nitrogen (Figure 15). As such, the electron count for the nitrogen is 12 (*i.e.* 5 + 6 + 1). Since this is four electrons more than the desired octet, it is evident that it is necessary to move two pairs of bonding electrons to the outer oxygen atoms. So doing results in the electron count of the nitrogen being decreased stepwise form 12 to 10 to 8, with the formal charge of nitrogen ultimately becoming +1, while two of the oxygen atoms adopt formal charges of –1.

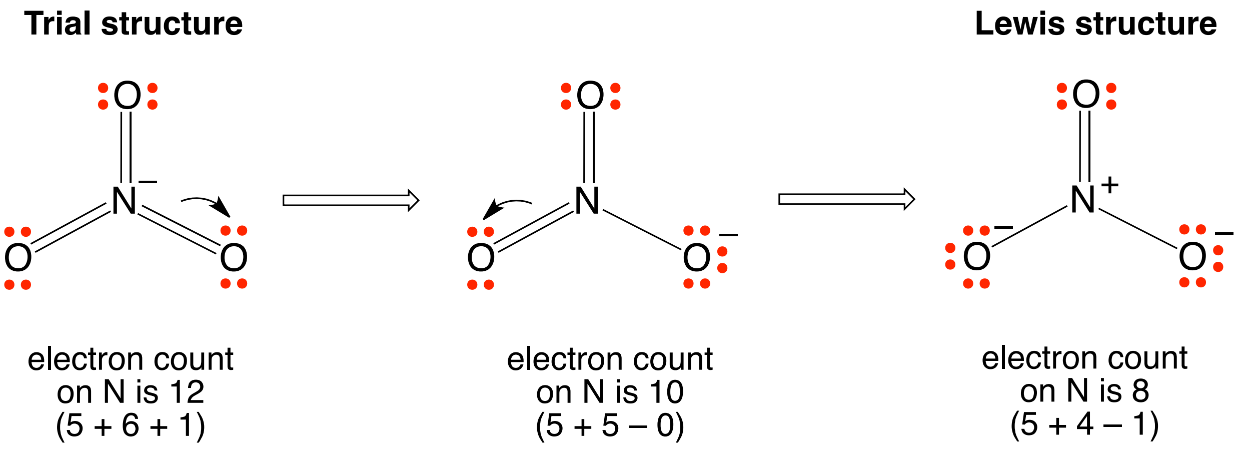

Figure 15. Trial structure for $[NO_3]^-$ obtained by drawing two bonds from the outer oxygen atoms to the central nitrogen atom and placing the negative charge on nitrogen (left). The nitrogen atom has an electron count of 12 and moving a bond pair to a lone pair on the oxygen atom results in a dectet configuration (center). The transfer of a second bond pair to a lone pair on oxygen is required to achieve an octet configuration, with a Lewis structure that has a formal positive charge on nitrogen and negative charges on two oxygen atoms (right).

The same procedure can be used for other oxo compounds, *e.g.* $[ClO_3]^-$ and $[ClO_4]^-$. Thus, even though an initial trial structure may have an apparently high electron count, it is trivial to reduce the trial structure to one that satisfies the octet rule by recognizing that each transfer of a bond pair to a lone pair lowers the electron count of the central atom by two. In this regard, if an initial trial structure has an electron count of N, the number of bonds that need to be transferred is $(N – 8)/2$ and this can be performed in a single step if one so desires, and so the process is direct and not arduous, as illustrated for $[ClO_3]^-$ in Figure 16.

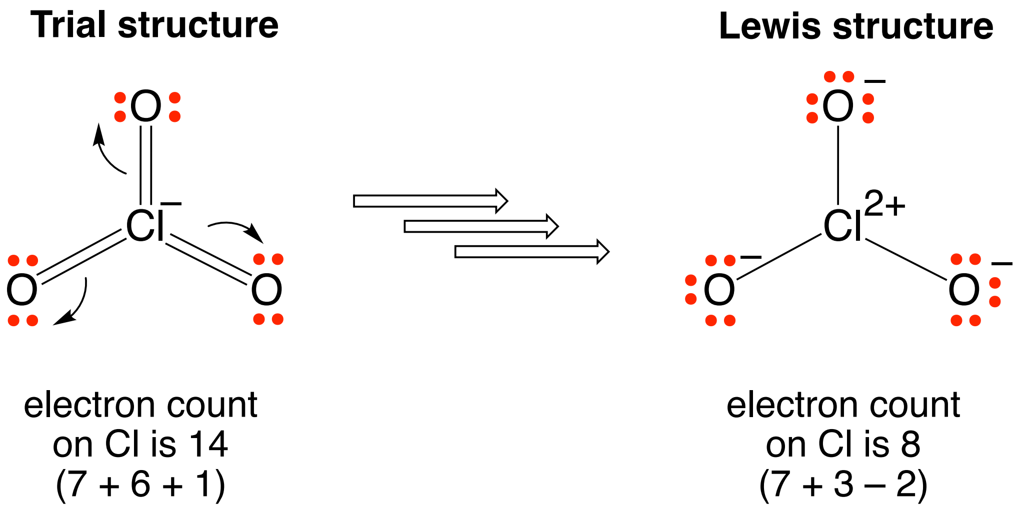

Figure 16. Trial structure for $[ClO_3]^-$ obtained by drawing two bonds from the outer oxygen atoms to the central chlorine atom and placing the negative charge on chlorine (left). The chlorine atom has an electron count of 14 and thus requires three electron pair bonds to be transferred to the outer oxygen atoms to achieve a Lewis structure with an octet configuration (right).

Examination of the Lewis structures of anionic $[NO_2]^-$ (Figure 14), $[NO_3]^-$ (Figure 15) and $[ClO_3]^-$ (Figure 16) indicate that the formal negative charges are localized on oxygen atoms that have single bonds to the nitrogen atoms. As noted above, this is a commonly observed motif for oxygen (Figure 5). Recognizing this fact, a student that is familiar with this observation could produce a trial structure for an oxyanion $[YO_n]^{Q-}$ (*e.g* $[CO_3]^{2-}$, $[SO_3]^{2-}$ and $[SO_4]^{2-}$) that features a negative charge on oxygen and the oxygen atom attached to the central atom by a single rather than double bond (for example, as illustrated by the central structure of Figure 15. However, it is recommend that this suggestion is only introduced to a student once they are proficient with the approach in which the charge is initially located on the central atom.

Hypovalent Trial Structures

The examples discussed above in which the trial structures are incorrect are those in which one of the atoms has an apparently expanded octet, which may be rectified by moving a bonding pair of electrons to a lone pair. In rare cases, however, an atom in a trial structure may have an electron count that is less than an octet configuration (*i.e.* hypovalent). One such example is provided by CO. Specifically, viewing oxygen as the outer atom, the carbon atom in CO has only a sextet configuration in the trial structure (Figure 17).

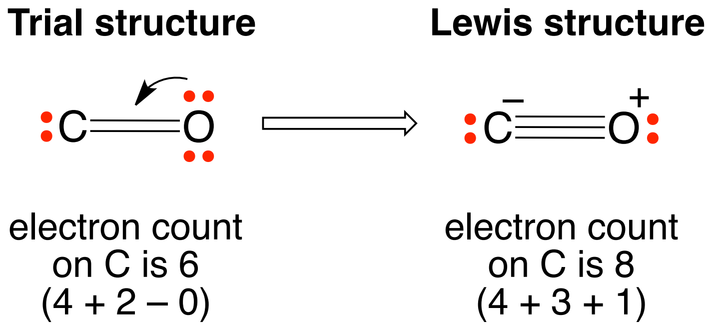

Figure 17. Trial structure for CO obtained by drawing two bonds from oxygen to carbon (left), which has a sextet configuration for carbon. Transferring a lone pair of electrons from oxygen to form a C–O dative bond achieves an octet configuration at carbon to arrive at the correct Lewis structure (right). Note how the formal charges on carbon and oxygen appear automatically and require no further calculation.

The situation is, nevertheless, readily rectified by recognizing that the oxygen atom can use one of its lone pair set of electrons to form an additional C–O bond *via* a dative interaction (Figure 6 and Figure 17). The transfer of a pair of electrons from oxygen to carbon not only results in carbon achieving an octet configuration, but also results in carbon adopting a negative formal charge and oxygen a positive formal charge. While these charges do not correspond to the electronegativities of these elements, it is important to emphasize that this is a common occurrence and that formal charges often do not correlate with those based on electronegativity.[15] The formation of a positive formal charge on oxygen and a negative formal charge on carbon upon utilizing a lone pair on oxygen to form a C–O bond is closely related is to the formal charges that are created on the nitrogen and boron atoms of H_3NBH_3 upon adduct formation (Figure 18). Note that the bond between boron and nitrogen can also be represented as a dative bond by using an arrow, in which case the formal charges are not included in the modified Lewis structure; however, despite their different appearance, the two structures describe the same electronic structure.[15]

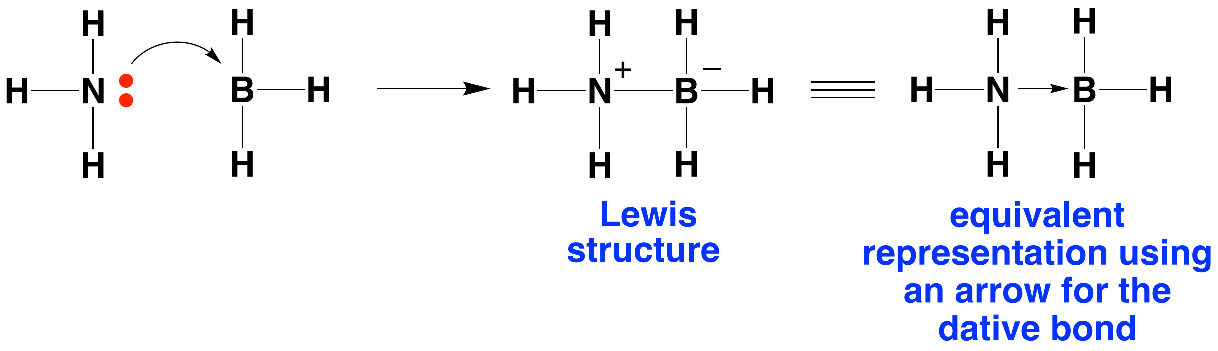

Figure 18. Creation of formal charges upon formation of a dative bond between two molecules, which can be represented as (i) a conventional Lewis structure with a line between N and B and formal charges and also as (ii) a modified Lewis structure that features a dative arrow.

A novel feature of the Lewis structure of CO is the presence of a lone pair on the carbon atom. This is not at all a common feature of carbon compounds, but is responsible for its ability to serve as a ligand for transitions metals.

The approach described here can also be used for radicals, with the recognition that it is not possible for all atoms to achieve an octet configuration. For example, NO would be represented with an N=O double bond in the trial structure, which would result in a septet configuration at nitrogen with three nonbonding electrons (Figure 19). While the electron count at nitrogen could be increased by lone pair donation from oxygen, as observed in CO, this would result in an expanded octet (9 electrons) and so is not considered to be a viable Lewis structure.

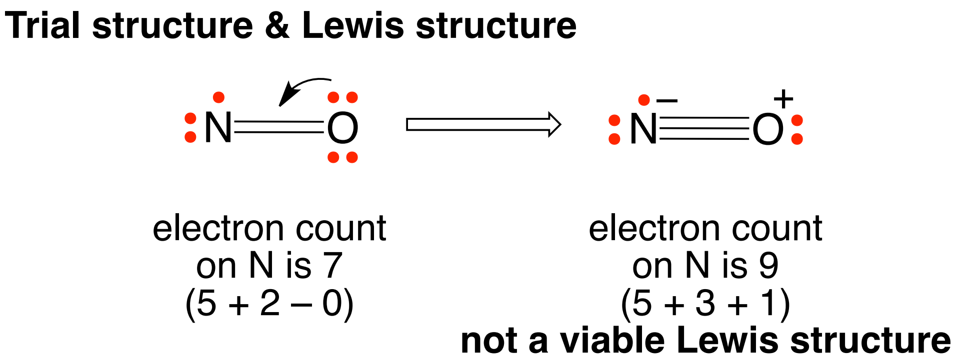

Figure 19. Trial structure for NO obtained by drawing two bonds from oxygen to nitrogen (left), which has a septet configuration for nitrogen. Transferring a lone pair of electrons from oxygen to form a N–O dative bond results in an expanded octet configuration at nitrogen (9 electrons), which is not a viable Lewis structure.

Lewis Structures for Elements of the Third and Subsequent Periods

In contrast to the second period elements, certain compounds of third and subsequent period nonmetals, such as PF_5, SF_6 and XeF_2, are often represented in basic chemistry texts with Lewis structures that have expanded octets, appealing to the notion that these elements utilize their *n*d orbitals in forming the bond. Such compounds are typically referred to as being hypervalent.[14] However, it has long been recognized that this bonding description is incorrect and that the compounds do indeed adhere to the octet rule.[14] Lewis structures for such compounds can also be obtained by using the procedure described herein.

For example, consider XeF_2. The trial structure, consisting of xenon forming single bonds to two fluorine atoms, corresponds to a dectet configuration for xenon. As discussed above for O_3, the situation can be rectified by converting a Xe–F bond into a lone pair on fluorine. The difference with O_3, however, is that the trial structure for O_3 possesses O=O double bonds and so cleaving a bond results in a structure that still features an O–O single bond (Figure 9). In contrast, cleaving a Xe–F bond results in a [F–Xe^+ F^-] species in which there is no covalent bond between xenon and one of the fluorine atoms (Figure 20); however, since there are two Xe–F bonds, this is only one possible resonance structure and so the Xe–F covalent bond order is formally 0.5 (Figure

21). In the context of molecular orbital theory, this situation is referred to as 3-center 4-electron bonding,[14] and reflects the fact that not all interactions between atoms can be described as simple 2-center 2-electron bonds.

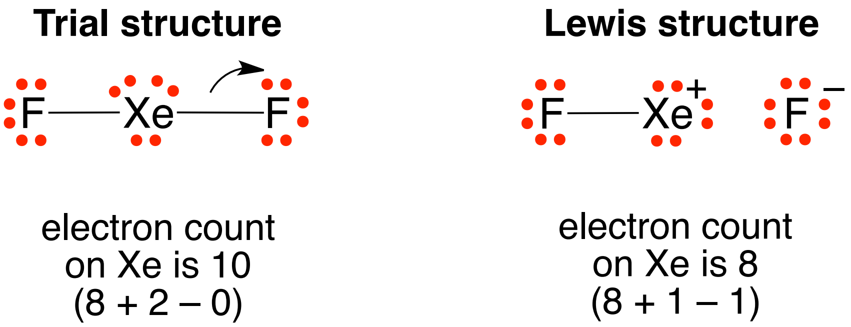

Figure 20. Trial structure for XeF_2 obtained by drawing single bonds from the outer fluorine atoms to the central xenon atom (left). The xenon atom has a dectet configuration and moving a bond pair to an outer fluorine atom, thereby becoming a lone pair, results in an octet configuration for xenon.

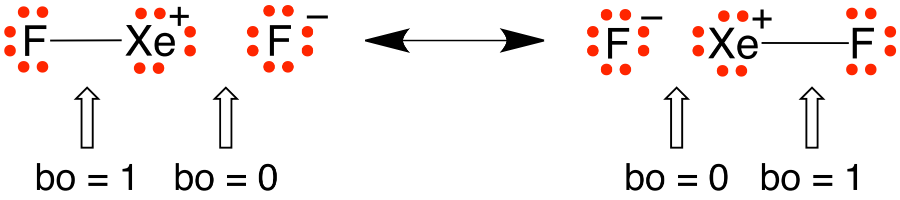

Figure 21. Two resonance structured for XeF_2 corresponding to a formal covalent bond order of 0.5.

Lewis Structures for Extended Molecules

The approach described above has focused on molecules in which there is either a clearly identifiable central atom or the molecule is diatomic. However, once a student masters the ability to draw Lewis structures for these molecules, it is a straightforward matter to apply it to molecules that have extended motifs. For example, consider nitric acid, HNO_3, or more precisely, $O_2N(OH)$. Recognizing that a neutral oxygen atom forms two bonds, the trial structure would feature the nitrogen being attached to (i) the OH group by a single bond and (ii) two oxygen atoms by double bonds (Figure 22).

Evaluation of the electron count of nitrogen in this trial structure indicates that it possesses 10 electrons. Therefore, one of the bonds of an N=O group needs to be relocated as a lone pair on oxygen, resulting in a formal positive charge on nitrogen and a formal negative charge on oxygen, with an octet configuration for nitrogen.

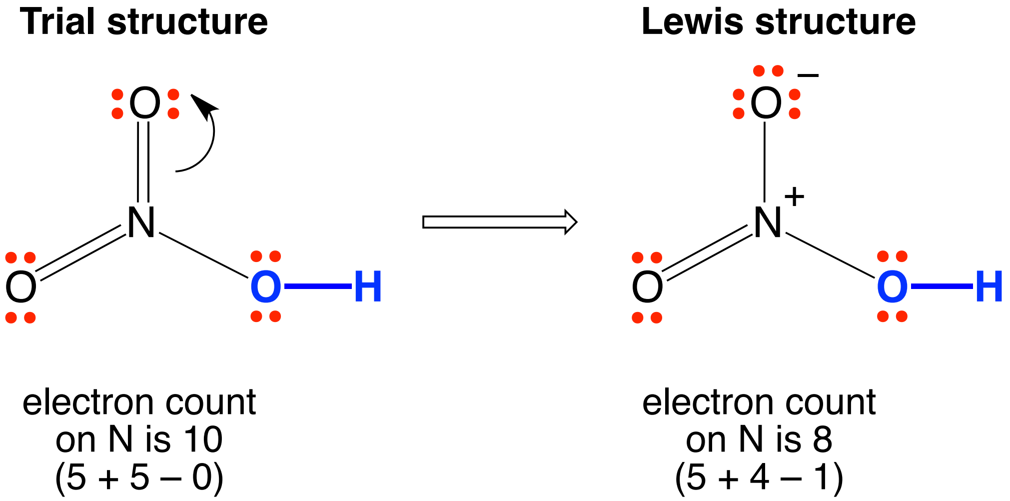

Figure 22. Trial structure for HNO_3 obtained by drawing double bonds from the outer oxygen atoms to the nitrogen atom and a single bond from the OH group to the nitrogen atom, each one being a consequence of the fact that a neutral oxygen atom forms two bonds (left). The nitrogen atom of the trial structure has an electron count of 10 and moving a bond pair from a N=O moiety to a lone pair on the oxygen atom results in an octet configuration (right). The transfer of a bond pair to a lone pair on oxygen results in an octet configuration for nitrogen with a formal positive charge on nitrogen and a formal negative charge on oxygen (right).

Concluding Remarks

In summary, a convenient approach to obtain a Lewis structure for a molecule involves (i) the initial construction of a trial structure that satisfies the valence of the outer atoms and placing the molecular charge (if any) on the central atom, followed by (ii) interconverting bond pairs and lone pairs to achieve an octet configuration for the central atom. This procedure results in the automatic generation of formal charges without the need to perform any additional calculation, and so is overall less likely to create erroneous structures as compared to more mathematical methods that focus on combining all valence electrons and then redistributing them.

As mentioned above, a plethora of methods exist for drawing Lewis structures. Although most descriptions involve summing all valence electrons in the first step,[9] some do not.[11] For example, some methods focus on drawing trial structures in which all atoms are attached by single bonds and the atoms are assigned lone pairs[11d] or formal charges[11e,f] that are determined by the number of bonds attached. In contrast to the approach used here, however, the sum of the formal charges of such a trial structure does not necessarily correspond to the charge on the molecule.[11e,f] As an illustration, the trial structure of the carbonate anion, $[CO_3]^{2-}$, has a formal negative charge on each atom such that the sum of the charges is –4 rather –2.[11e,f] In contrast, the sum of the formal charges of the trial structure for the method described here will necessarily be equal to that of the molecule, which is a distinct advantage.

The approach presented here has been taught in a section of a General Chemistry I course at Columbia University since 2006. Students that have taken this course have subsequently commented that, when they take Organic Chemistry I, they feel more adept at drawing structures of molecules than do their colleagues who took a different section of General Chemistry I.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available on the ACS Publications website at DOI: 10.1021/acs.jchemed.XXXXXXX.

Examples of erroneous Lewis structures (PDF).

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Notes

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