A Simple Approach for Beginners to Drawing Lewis Structures, Resonance Forms, and Isomers

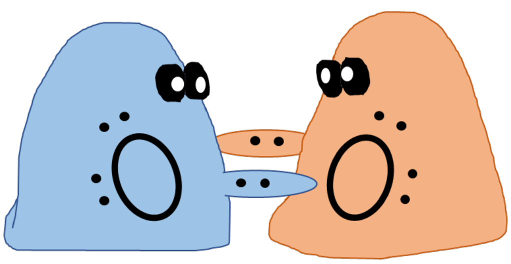
Qi Cui, Jordan Harshman*

Department of Chemistry & Biochemistry, Auburn University, Auburn, AL 36849, United States

ABSTRACT

Lewis structures, resonance forms, and isomers are difficult for beginners to draw in a general chemistry class. Though various methods and their improved procedures have appeared in the literature and general chemistry textbooks, most of them are too complicated to understand or can only be applied to a small number of molecules. A simplified approach with the rationale behind it for drawing Lewis structures, resonance forms, and isomers is introduced in this paper. In addition, the adjusted procedures that deal with odd-electron molecules or ions are also proposed.

GRAPHIC ABSTRACT



KEYWORDS

First-Year Undergraduate/General, Curriculum, Lewis Structures, Resonance Theory

INTRODUCTION

Lewis structures, also known as electron-dot structures, are diagrams that represent how the electrons are arranged around each atom in a molecule or ion. Drawing Lewis structures is an important skill that students need to acquire in the introductory chemistry curriculum. It is the starting point for understanding and predicting some physical and chemical properties, such as molecular geometry using the Valence Shell Electron Pair Repulsion Theory (VSEPR), acidity and basicity, reactivity, polarity, intermolecular forces, and solubility etc.[1-8]

However, a number of studies stated that students had difficulties drawing Lewis structures.[3-6, 9-16] Lever[10] mentioned the confusion about writing the correct number of multiple bonds when students drew a Lewis structure. Additionally, Cooper et. al[16] noted that drawing Lewis structures was more difficult for students in the following circumstances: (a) increased molecular complexity, such as change from one- to two-carbon species, and (b) the formula was presented without structural cues even for some simple molecules.

In order to help students draw Lewis structures correctly and easily, various approaches have appeared in the research literature and general chemistry textbooks.[1-4, 9-15, 17-24]

Lever[10] proposed "6N+2" rule for noncyclic molecules, in which the number of π bonds can be determined by the total number of valence electrons and the total number of atoms in a molecule. Following this proposed rule, Clark[12] provided detailed procedures for writing Lewis octet structures without understanding σ or π bonding. In the same year, Zandler & Talaty[2] listed more examples to account for more types of species, such as cyclic molecules. However, the rule is not applicable to non-octet Lewis structure or odd-electron structure.

Pardo[1] created another method for drawing Lewis structures using the total number of valence electrons and the total number of electrons needed for octet to identify the σ and π bonds. However, students are generally taught Lewis structures prior to really learning what σ and π bonds refer to, delineating bonds as σ or π would be conceptually difficult for students.

Similarly, Miller developed guidelines[18] that call for distributing the bonding electrons to atoms to form single bonds or multiple bonds. This is followed by dividing total valence electrons to bonding and nonbonding electrons. Alternative procedures were presented by Mortimer, Davis, Gaily[19], Ahmad & Omar[3], and Whitten[20], these procedures follow the strict octet rule and cannot be applied to free radicals. In addition, the procedures are complicated and require iterative calculations when molecular complexity increases, so that it is likely to make mistakes for beginners when writing the Lewis structures.

The approach introduced by Carroll[9] requires only the number of valence electrons rather than the octet rule. When drawing a Lewis structure, all electrons are assigned to atoms in pairs to form bonds or lone pairs. He stated that the structure with more bonds or less formal charges tends to be more important. However, it is used only for even-electron molecules. Moreover, the octet rule is a fundamental concept in general chemistry curriculum, it is essential to be taught in the class.

Recently, an approach was outlined by Nassiff and Czerwinski[4]. They emphasized that students follow the summarized table to find the difference between the number of valence electrons required and the number of valence electrons in the complete octet. The examples they introduced are only molecules or ions with specific AB_X format and strictly following the octet rule.

The most recent study of constructing Lewis structures was presented by Curnow[25]. The author described a method to determine formal charges of main group elements without counting the total valence and checking the Lewis structures by formal charge formulas. The procedure is based on the knowledge of the element's position in the periodic table and the number of electrons to form an uncharged molecule. However, relatively complicated formal charge calculation as the first step may lead to the wrong Lewis structure construction from the beginning.

Some other methods or rules[11, 15, 21-23] either describe simple but inadequate procedures or are too complicated and difficult for beginners to understand. To deal with the difficulties[10, 16, 26] students encountered, a simplified method for drawing Lewis structures, resonance forms, and isomers for molecules or ions is introduced. To expand the use of this method, the adjusted procedures to deal with the odd-electron molecules are also proposed herein.

RATIONALE

Assuming that circles A and B represent two datasets, respectively. $C = A \cap B$, is the intersection of these two datasets, and dataset $D = A - C$; $F = B - C$. Thus, $A + B = (D + C) + (F + C) = (D + C + F) + C$ (Figure 1)

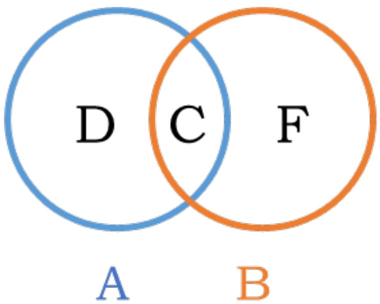


Figure 1 Simple model for molecules with two atoms

Thinking about a molecule and its Lewis structure, let's assume that D and F are lone pair electrons around atoms A and B, while C is the number of bonding electrons. D + C + F is the total number of valence electrons in a molecule; D +C and F + C are both the numbers of electrons needed to complete the octet (duet for hydrogen) for each atom. Thus, the difference between the total electrons needed for the octet and the total valence electrons indicates the number of bonding electrons. As two bonding electrons form one chemical bond, the number of bonds formed by every two electrons can be determined.

The following generalized model for molecules/ions with multiple atoms is provided below to show how one can easily calculate the bond number for the molecule, which is used to determine the number of single, double, and triple bonds in molecules. (Figure 2)

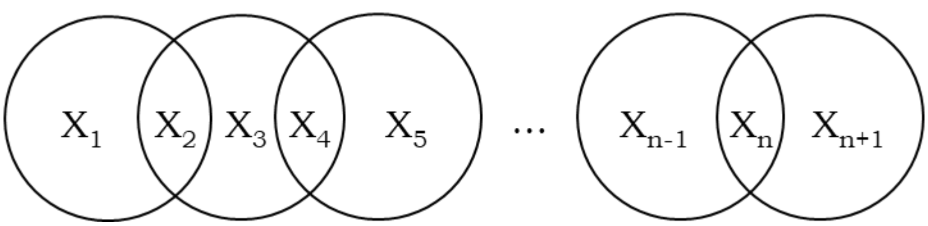


Figure 2 Generalized model for molecules with multiple atoms

(1) The number of lone pair electrons surrounding each atom = $X_1 + X_3 + X_5 + \ldots + X_{n-1} + X_{n+1}$

The number of bonding electrons = $X_2 + X_4 + \ldots + X_n$

(2) The total number of valence electrons = $X_1 + X_2 + X_3 + X_4 + X_5 + \ldots + X_{n-1} + X_n + X_{n+1}$

(3) The total number of electrons needed for all atoms to complete the octet

$= (X_1 + X_2) + (X_2 + X_3) + (X_3 + X_4) + (X_4 + X_5) + \ldots + (X_{n-1} + X_n) + (X_n + X_{n+1})$

$= (X_1 + X_2 + X_3 + X_4 + X_5 + \ldots + X_{n-1} + X_n + X_{n+1}) + (X_2 + X_4 + \ldots + X_n)$

(4) Difference between (3) & (2) = Bonding electrons = $X_2 + X_4 + \ldots + X_n$

(5) Bond number = $(X_2 + X_4 + \ldots + X_n)/2$

PROCEDURES

General procedures:

(1). Select an appropriate skeletal atom arrangement for a chemical formula. The central atom would be the atom that is with the least number and electronegativity in a formula. The period III-IV nonmetal element should be present as a central atom. The atoms, H and F, occupy the peripheral position in any polyatomic molecule or ion. If there are different reasonable atom arrangements, they represent isomers.

(2). Count the total number of valence electrons in the species by adding together the numbers of valence electrons of each atom. For each anion/cation, the number of electrons that equals to the charge should be added/subtracted.

(3). Calculate the total number of electrons (E) needed to complete the octet with all the atoms in the molecule or ion by eq.1. In the case of existing hydrogen atoms, two electrons will be added to each of these atoms instead of eight.

$E = 8e^- \times M + 2e^- \times N$ eq.1

M = the total number of non-hydrogen atoms; N = the total number of hydrogen atoms

(4). The number of bonding electrons (shared electrons) is determined by (3) - (2)

(5). As two bonding electrons form one chemical bond, the number of bonds formed by every two electrons can be determined by eq.2.

Bond number = The number of bonding electrons /2 = (4) / 2. eq.2

(6). List all possible bond number combinations based on the type and the number of peripheral atoms.

Bond number = (5) = $A_1 + A_2 + A_3 + \ldots + A_K$ eq.3

$K = M + N - 1$;

A_1, A_2 … A_K are bond numbers that can be chosen from 1 (single bond), 2 (double bond), and 3 (triple bond).

Note that hydrogen and halogen atoms are assumed to form single bonds only, so $A_K = 1$. Thus, if there are hydrogen or halogen atoms present in a molecule, the bond number will subtract the number of these peripheral atoms, then list all possible combinations of the rest bond number.

For example, the total bond number calculated by procedure (1)-(5) for C_2H_4O is $7 = A_1 + A_2 + A_3 + A_4 + A_5 + A_6$. There are 4 hydrogen atoms ($A_1 + A_2 + A_3 + A_4 = 1 + 1 + 1 + 1 = 4$), then we only need to list the possible combination of the rest bond number, which is 7 - 4 = 3. Thus, the two bonding spots between C, C, and O are single bond & double bond (3 = 1 + 2), or double bond & single bond (3 = 2 + 1).

(7). Complete the octets on each atom (duet on hydrogen) for all the possible structures, which represent different resonance forms.

(8). To check for the preferred resonance form, the formal charges on each atom in all proposed structures should be taken into consideration. A preferable Lewis structure is the one where more atoms have formal charges of zeros and negative formal charges should be on the more electronegative atoms.

Odd-electron molecules disobey the octet rule. Thus, the adjusted procedures are proposed to handle some of these cases.

Adjusted procedures for some cases that violate octet rule:

a. If the total number of valence electrons is odd, it represents the free radical. Then step (4) will be adjusted to (4)a and step (7) will be adjusted to (7)a.

(4)a. The number of bonding electrons (shared electrons) is (3) – (2) -1, because one single electron is not able to form a chemical bond.

(7)a. Complete the octets on all atoms (duet on hydrogen) except one atom filled with the rest of the electrons for all possible structures.

EXAMPLES

The procedures introduced above can be applied to a variety of examples, including diatomic molecules, polyatomic species, complex ions, free radicals.

Example 1: O_2

(1). Atom arrangement

O O

(2). Total number of valence electrons = $6e^-$ (O) x 2 = $12e^-$

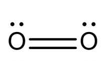
(3). The number of total electrons needed to complete the octet =$8e^-$ x 2 = $16e^-$ (M = 2)

(4). The number of bonding electrons = $16e^-$ - $12e^-$ = $4e^-$

(5). Bond number = $4e^-/2$ = 2 bonds (double bond)

(6). Only one bonding spot (K = 2 -1 = 1), meaning only one possible combination, skip this step

(7). Complete octets on each atom:



(8). There is only one Lewis structure of O_2, skip this step.

Example 2: CN^-

(1). Atom arrangement

C N

(2). Total number of valence electrons = $4e^-$ (C) + $5e^-$(N) + $1e^-$ (anion) = $10e^-$

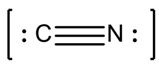
(3). The number of total electrons needed to complete the octet = $8e^-$ x 2 = $16e^-$(M = 2)

(4). The number of bonding electrons = $16e^- - 10e^- = 6e^-$

(5). Bond number = $6e^-/2$ = 3 bonds (triple bond)

(6). Only one bonding spot (K = 2 -1 = 1), meaning only one possible combination, skip this step

(7). Complete octets on each atom:



(8). There is only one Lewis structure of CN^-, skip this step.

Example 3: CO_2

(1). Atom arrangement

O C O

(2). Total number of valence electrons = $4e^-$(C) + $6e^-$ (O) x 2 = $16e^-$

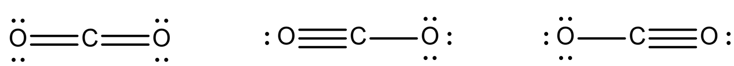
(3). The number of total electrons needed to complete the octet = $8e^-$ x 3 = $24e^-$ (M = 3)

(4). The number of bonding electrons = $24e^- - 16e^- = 8e^-$

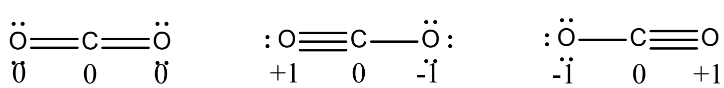
(5). Bond number = $8e^-/2$ = 4 bonds

(6). There are two bonding spots, K = 3 – 1 = 2. All possible combinations: 4 = 2 + 2; 3 + 1; 1 + 3. Thus, there should be three resonance forms for CO_2.

(7). Complete octets on each atom for all the possible structures.

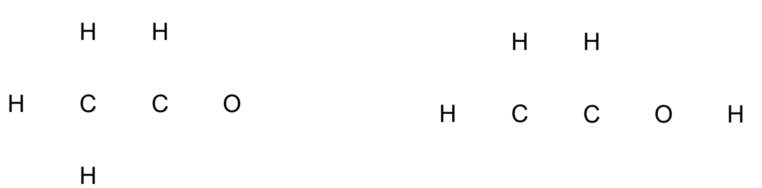


(8). Check for the formal charges on each atom, and the structure with zeros on all atoms is the best representative for CO_2.



Example 4: C_2H_4O

(1). Atom arrangement:



There are two reasonable atom arrangements, they indicate two isomers for this chemical formula.

(2). Total number of valence electrons = $4e^-$(C) x 2 + $1e^-$(H) x 4 + $6e^-$(O) = $18e^-$

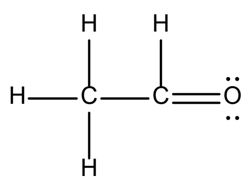
(3). The number of total electrons needed to complete the octet = $8e^-$ x 3 + $2e^-$ x 4^- = $32e^-$ (M = 3; N = 4)

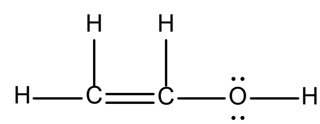
(4). The number of bonding electrons = $32e^-$ - $18e^-$ = $14e^-$

(5). Bond number = $14e^-/2$ = 7 bonds

(6). Hydrogen atoms can only form single bond, thus there are only 7 – 4 = 3 bonds can be varied in the combinations: 3 = 1 + 2; 2 + 1. Thus, there should be two forms for CH_3CHO.

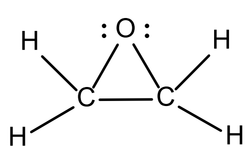
(7). Complete octets on each atom (duet on hydrogen) for all the possible structures.





(8). The formal charges on all atoms in these two structures all equal to zero, these two structures are isomers.

It is worth noting that for upper-level chemistry courses where epoxides would be introduced, the epoxide ring arrangement is one of the possible arrangements in addition to the straight-chain Lewis structures described above. As the calculated total bond number is 7 and four hydrogen atoms can form four single bonds, the only possible ring arrangement of C_2H_4O is ethylene oxide which forms three single bonds between C, C, and O. The formal charges on all atoms in the structure equal to zero, this is a stable compound.



Example 5: NO

(1). Atom arrangement

N O

(2). Total number of valence electrons = $5e^-$(N) + $6e^-$(O) = $11e^-$

(3). The number of total electrons needed to complete the octet = $8e^-$ x 2 = $16e^-$ (M = 2)

(4)a. Odd-electron molecule, the step (4) is adjusted to (4)a

The number of bonding electrons = (3) – (2) - 1 = $16e^-$ - $11e^-$ - $1e^-$ = $4e^-$

(5). Bond number = $4e^-/2$ = 2 bonds (double bond)

(6). Only one bonding spot (K = 2 -1 = 1), meaning only one possible combination, skip this step

(7)a. Complete octet on one atom, leaving the other atom filled with the rest electrons for all possible structures.

(8). Check for the formal charges on each atom, and the structure with zeros on both atoms is the best representative for NO.

CONCLUSION

The method proposed in this paper is simple for beginners to draw an appropriate Lewis structure, its resonance forms, as well as isomers. The algorithm is based on straightforward mathematical calculations and is easy to understand for beginners, especially when the molecular complexity increases because the number of multiple bonds in a molecule is easy to be determined by this approach. The approach is the direct application of the octet rule. However, it can also be applied to various species violating the rule, such as some types of odd-electron molecules or ions. In addition, it does not require σ/π concept prior to Lewis structures, so that students will not have conceptual difficulties when using this method.

The procedures introduced here are expected to provide an alternative to teaching Lewis structures for beginners, but not meant to be exhaustive for all molecules. For example, the central atom sulfur may exhibit an expanded octet to reduce high formal charges in the octet structure of SO_4^{2-}. The non-octet structure for SO_4^{2-} cannot be drawn by this proposed method. Other exceptions include PO_4^{3-}, $POCl_3$ etc. These non-octet structures remain challenging for teaching using the recent reported methods, as there is no clue for beginners to figure out which is the exception. It would need further studies.

STUDENT FEEDBACK

While we have not formally gathered evidence of the efficacy of this activity, we noted experiences using this method from twenty first-year university students in a formal tutoring environment as well as review sessions of General Chemistry I. These students had learned the traditional method for constructing Lewis structures in the classroom settings. Anecdotally, we found that students quickly adopted and implemented the method in their studies and we did not detect significant struggles in understanding the conceptual basis behind it. At minimum, we hope this novel method could be used at least as a supplement to existing methods for determining appropriate Lewis structure.

AUTHOR INFORMATION

Corresponding Author

Jordan Harshman – Department of Chemistry & Biochemistry, Assistant Professor, Auburn University, Auburn, AL 36849, United States orcid.org/0000-0003-0783-465X Email: jharshman@auburn.edu

Author

Qi Cui – Department of Chemistry & Biochemistry, Graduate Research Assistant, Auburn University, Auburn, AL 36849, United States orcid.org/0000-0002-3034-1143 Email: qzc0009@auburn.edu

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