Facile Method for Constructing Lewis (Electron Dot) Structures

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ABSTRACT: A simple method to determine Lewis electron dot structures and formal charges without a need to sum all of the valence electrons, reorganize electron pairs, draw and pair up individual electrons, or remember a formal charge formula is described. The formal charge is determined by the group number (number of valence electrons) and the number of bonds, with the sum of formal charges then being equal to the total charge. This leads directly to a valid Lewis structure. The facility of the procedure allows the student to focus more on the chemical aspects of deciding which valid Lewis structure (or structures) is the correct or most important one.
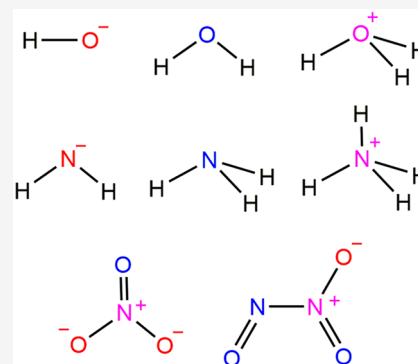
KEYWORDS: *Lewis Structures, First-Year Undergraduate/General, High School/Introductory Chemistry, Curriculum*

INTRODUCTION

Lewis electron dot structures are critical to our rationalization of the structures and chemistry of the p-block elements. The early work by Lewis, Pauling, and others in this area is fundamental to our modern understanding of chemistry.[1,2] However, as stated by Lever in 1972: "Until expertise has been gained, confusion often arises concerning the correct number of multiple bonds to use, the correct number of valence electrons to use, and the placing of formal charges."[3] Since then, there has been a lot of research and discussion into the difficulties of drawing Lewis structures[4−14] as well as the development of a variety of procedures, or modifications to existing procedures.[4,5,15−28] Kaufmann et al. recently found that "it is possible to distinguish three main components to these procedures. At first, there is an initial element of construction: construct a Lewis structure by calculating the total number of valence electrons, draw the skeletal structure and distribute the remaining electrons."[6] Distribution of the remaining electrons is then done such that the octet rule is satisfied for each atom (except for H which normally has only two electrons). Following the initial construction, there is a checking step and, if necessary, a modification step or steps. Although the process is simple in principle, in practice, it is easy to miscount the electrons both during construction and during the checking and modification steps. Students frequently make mistakes and have to do multiple recounts as they rearrange and add or remove electron pairs. This can be both frustrating and time-consuming, especially for larger systems.

As already noted by Kaufmann, most procedures require a total valence electron count; however, a couple rely on a stepwise pairing process of valence electrons.[19−21] The procedure I will describe here does not require a total valence electron count, the drawing and pairing-up of individual electrons, or modification steps involving rearrangements of lone pairs (rearrangements of bonding pairs, however, readily provide a variety of valid Lewis structures). Furthermore, my procedure does not need a formal charge formula, or even the drawing of the lone pairs. Fundamentally, all that is required is a knowledge of each atom's position in the periodic table, which is essential knowledge required by any procedure and is what all chemical educators aim to reinforce anyway.

DISCUSSION

Rationalization and Determination of Formal Charge

Formal charge is a fundamental component to rationalizing the possible Lewis structures that might be constructed for a particular species, as well as for understanding many of the properties of these species. Importantly, formal charge is directly related to the number of valence electrons (i.e., their periodic properties) and the number of bonds (i.e., their structure). This method uses the fact that the sum of formal charges must be equal to the total charge in order to develop valid Lewis structures. The procedure is also related to the HONC 1234 rule
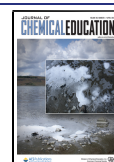
for drawing simple uncharged organic molecules in which H, O, N, and C have 1, 2, 3, and 4 bonds, respectively.

The method is constructed and rationalized on the basis of the determination of formal charge as follows: On the basis of the octet rule, carbon, from group 14 with four valence electrons, requires four more electrons to form an octet. It can do this by forming four covalent bonds, as each covalent bond adds one electron (shared with the other atom). The formal charge on the carbon atom will remain as zero, since each covalent bond contains an electron from each contributing atom. However, if the carbon atom only has three covalent bonds, then it will only have seven electrons, and we need to add one more electron to the carbon atom to complete its octet. The effect of this will be to give a carbanion, CR_3^-, with one lone pair and a formal charge of −1 (Scheme 1), similarly for nitrogen which needs three bonds

Scheme 1. Basic Structures for Compounds of Groups 14 and 15
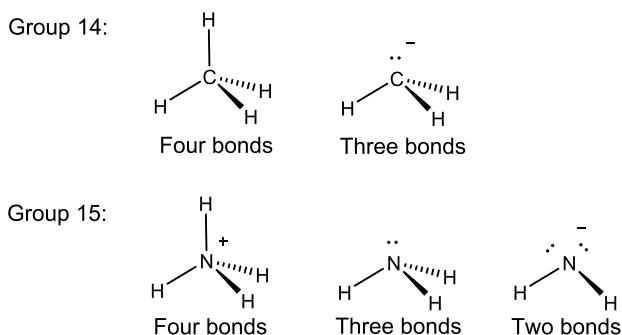
to achieve an octet with a formal charge on N of zero. Again, if it is missing a bond, it will require an extra electron and will have a formal charge of −1, e.g., amide, NH_2^-. On the other hand, if it has an extra bond (four bonds in total), it must lose an electron to maintain its octet, and so N will have a formal charge of +1, e.g., ammonium, NH_4^+. The formal charge determination will apply similarly for other members of groups 14 and 15.

It should be obvious now that oxygen will require two bonds for a formal charge of zero on oxygen (e.g., water, H_2O); losing one bond gives a −1 formal charge (hydroxide, OH^-), and losing both bonds gives a −2 formal charge (oxide, O^{2-}). The halogens require one bond (X_2) and will form a halide (X^-) if they have no bonds. Naturally, elements in the same group will follow the same rules for determining the formal charge. Determining the formal charge for elements that obey the octet rule is now very simple and is summarized in Table 1. One does not need to remember Table 1, only the number of bonds that each group needs for zero formal charge. Note that boron, with three valence electrons, cannot form five covalent bonds but must "lose" a bond to form a borate, BR_4^-, with a −1 formal

Table 1. List of the Number of Bonds Based on Formal Charge for p-Block Elements That Obey the Octet Rule

Formal Charge	Group 13	Group 14	Group 15	Group 16	Group 17
−3		1	0		
−2		2	1	0	
−1	4	3	2	1	0
0		4	3	2	1
+1			4	3	2
+2				4	3

charge. Electron deficient, radical, and hypervalent molecules obviously do not obey the octet rule; these are addressed in the Supporting Information.

Procedure

Molecules can now be constructed because the sum of the formal charges equals the total charge. The general procedure then becomes the following:

(i) Draw the molecular framework with one covalent bond between each atom and assign the formal charges;

(ii) Add bonds until the total charge is correct (ensuring that no atom has more than 4 bonds);

(iii) Place lone pairs so that every atom has an octet.

This can be summarized as draw the skeletal structure and add bonds until the formal charges add up to the molecular charge. Note that each additional bond will increase the sum of formal charges by +2. If the sum of the formal charges differs from the actual charge by an odd number, then the species will be a radical, and if it is greater than the actual charge, then it is a hypervalent molecule (see Supporting Information).

Examples

Consider carbonate, CO_3^{2-}. After step i, it will look like **A** in Scheme 2. This structure assumes that each atom obeys the octet

**Scheme 2. Construction of the Lewis Structure for CO_3^{2-}**
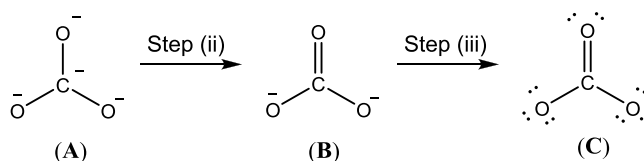
rule; however, it is an incorrect structure because the sum of formal charges is −4 rather than −2 (lone pairs do not need to be drawn at this stage as this structure does not yet have a correct bonding framework). Addition of one bond, step ii, will increase the formal charge by +2 to the correct value of −2 and thus generate a valid Lewis structure (**B**). The lone pairs can now be placed, step iii, in accordance with the octet rule (**C**). After very little practice, most will find it easier and quicker to start by making as many atoms as possible have the number of bonds that gives them zero formal charge, and to adjust the structure from there. The Supporting Information gives examples of alternative structures that are valid but incorrect and discusses why they are incorrect.

When there are a number of possible valid Lewis structures, we minimize formal charges and keep negative charges on the more electronegative atoms. The procedure described here facilitates the decision-making process since the formal charges are quickly determined (without having to use the formal charge formula: valence electrons − bonds − unshared electrons). Thus, this procedure also makes it easy to quickly compare a set of valid Lewis dot structures, as would be found in thiocyanate, NCS^-, for example (Scheme 3). Structure **A** has low formal charges, and the negative charge is on the most electronegative

Scheme 3. Three Valid Lewis Structures for SCN^-
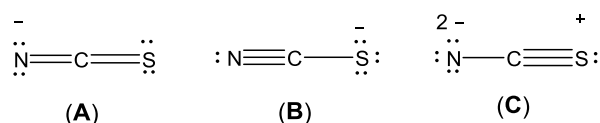
Scheme 4. Which Is the Correct Lewis Structure for SO₂?
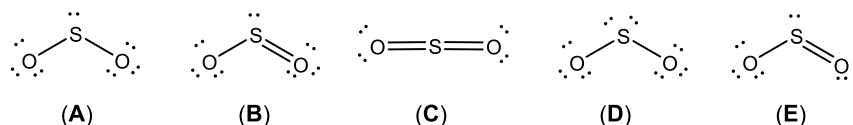
atom; however, a C=S double bond is not very strong. In structure **B**, although the negative charge is not on the most electronegative atom, CN multiple bonds are very strong. Structure **C** has large formal charges and a relatively weak C≡S triple bond. Thus, **A** and **B** are the important resonance structures of NCS^-.

Testing Lewis Dot Structures

The method also makes it easier to identify incorrect Lewis structures. Consider some possible Lewis structures for SO_2 in Scheme 4. Structures **A** and **B** are easily identified as being incorrect because there are atoms that do not obey the octet rule. In structures **C** and **D**, however, each atom has an octet, and to test whether they are correct or not would require counting all of the electrons. Alternatively, using the method described here, **C** is easily identified as being the structure of nonexistent SO_2^{2+} (since an S atom with four bonds would have a formal charge of +2), and **D** is the structure of nonexistent SO_2^{2-} (since each O atom with one bond would have a formal charge of −1). Structure **E** has a negative charge on one O atom (with the single bond) and a positive charge on the S atom (with three bonds), for an overall charge of zero; all atoms obey the octet rule, and it is therefore correct.

Implementation in a Teaching Context

Within a chemistry curriculum, whether it be in high school or during the first year of university, there are a number of topics that need to be covered before Lewis structures are discussed, no matter which method is used. In particular, simple atoms and ions such as Ar, Na^+, and Cl^- would be discussed to introduce the octet rule and the number of valence electrons based on group number; simple molecules such as F_2, O_2, N_2, H_2O, C_2H_4, etc. would be used to introduce covalent bonding, multiple bonds, and lone pairs, and for further reinforcement of the octet rule; electronegativity would also be introduced by using simple compounds such as H_2, HF, and NaCl. Formal charge, on the other hand, would normally be covered toward the end of the teaching of Lewis structures so as to decide upon the most plausible structure when there is more than one option. The procedure described here addresses formal charge at the beginning of teaching Lewis structures. Students should have early practice in determining the formal charges on simple compounds before trying to draw their own Lewis structures as described here for compounds that obey the octet rule. Exceptions such as electron deficient species, radicals, and hypervalent molecules can be, and often are, discussed much later in the curriculum. I have included these topics in the Supporting Information.

Having obtained a set of valid Lewis structures, other chemical principles can then be considered to predict and rationalize the actual structures and their properties. The following principles can be introduced when most appropriate (see the Supporting Information for examples):

- The most electropositive (non-hydrogen) atom usually goes in the middle;
- Formal charges should be minimized;
- Like charges should not be next to each other;

- Negative charge is preferred on the more electronegative atom;
- Multiple bonds are favored by small atoms of the first row (B to F), but one second row element (Si to Cl) in a multiple bond is reasonably strong;
- Small rings (3 or 4 atoms) are disfavored over larger rings due to ring strain;
- Atoms should be able to adopt their preferred geometry based on VSEPR.

Compared to the previously described methods referenced here, some advantages of this method are that

- The elimination of a total valence electron count significantly simplifies the procedure;
- There is less reorganization of electron pairs;
- Formal charges are more easily determined;
- There is more focus on chemical principles of stability.

Some of the advantages compared to the stepwise pairing processes that similarly do not require a total valence electron count[19−21] are that

- Individual electrons do not need to be drawn and individually paired up;
- Formal charges are easily and automatically generated;
- It is not necessary to decide where to put an extra electron in the case of a negative charge (or remove in the case of a positive charge).

Kaufmann et al. and Cooper et al. have discussed the challenges that students encounter in drawing Lewis structures, and I have detailed how I believe this procedure addresses those in the Supporting Information.[6,8]

■ CONCLUSIONS

I have described a simple method to determine formal charges of main group elements which then allows an easy method to construct Lewis structures. It should be recognized that this is simply a different way of counting electrons to satisfy the octet rule, so the resultant structures cannot be any different from what can be obtained by other procedures. With relatively little experience, students can quickly simplify the drawing procedure to three basic steps: Draw a structural framework, determine the formal charges, and add the appropriate number of bonds. I have provided a list of common and less common chemical principles to then determine the most likely, or significant, Lewis structures. This is probably not an exhaustive list.

The fact that the procedure is based on periodic properties of the elements means that it is useful as a way both to build Lewis structures and to develop strength in understanding periodicity and structure. Traditional methods require a total electron count and are thus focused on distributing those electrons. This method focuses on the properties of individual atoms and thus emphasizes periodic properties and how these affect their structure; this is a fundamental and primary goal of chemical educators. I believe that this method could solve many of the problems that students commonly have when drawing Lewis structures and is certainly appropriate to be taught at high school and university level.

STUDENT FEEDBACK

I introduce this method to first year university students as well as at the annual New Zealand Chemistry Olympiad camp for senior high school students. These students have all previously been taught the traditional method for drawing Lewis structures. I present both methods, but I find that a vast majority of students quickly adopt the method described here, despite their earlier introduction to the traditional method.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available at https://pubs.acs.org/doi/10.1021/acs.jchemed.0c00952.

> Molecules that do not obey the octet rule (electron deficient, radical, and hypervalent), further examples to illustrate chemical principles, summary of how the challenges of drawing Lewis structures are addressed, and some useful problems (PDF)

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Notes

The author declares no competing financial interest.

ACKNOWLEDGMENTS

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