Drawing Lewis Structures from Lewis Symbols: A Direct Electron Pairing Approach

Wan-Yaacob Ahmad* and Mat B. Zakaria
School of Chemical Sciences and Food Technology, Program of Chemical Sciences, Universiti Kebangsaan Malaysia,
43600 UKM Bangi, Malaysia; **wanyaa@pkrisc.cc.ukm.my*

Lewis structures for covalently bonded molecules and ions can be derived by pairing valence electrons in accordance to Lewis theory and Abegg's rule (*1*). Lewis theory dictates that a bond contains a pair of opposite spinning electrons each attracted by two adjoining atomic nuclei. Each bonded atom, at the same time, tends to mimic and attain a noble gas electronic configuration in which the outer shell possesses the octet state to satisfy the Abegg's rule. Various approaches to writing Lewis structures have been presented in general chemistry textbooks and journals (*2–13*). We have developed a different method of writing Lewis structures. Quantum mechanics, atomic orbitals, and the spdf electronic configurations are not a prerequisite. What is needed is merely the atomic position in the periodic table, since the number of outer-shell electrons equals the group number.

Our electron-pairing method has been used to a certain degree in many general chemistry textbooks, but usually is limited to molecules where the pairing is rather straightforward. Many students find it difficult to apply to some covalent entities, especially those having multiple resonance structures. Other approaches are more mathematical and the structures seem to have been derived without considering the periodic table, Lewis theory, and Abegg's rule. Our procedure gives Lewis structures rather directly and gives formal charges automatically.

Central Atom

A Lewis structure will be meaningless if the central atom is incorrectly designated (*15, 16*). The following are guidelines in selecting central atoms for species with a single layer of surrounding atoms.

1. A single atom in a formula is always the central atom. Thus the central atom for BF_3 would be B; for NO_3^-, N; for H_3O^+, O; for ClO_3^-, Cl; for XeF_4, Xe; for MnO_4^-, Mn; and for CrO_2Cl_2, Cr.
2. For species containing two or more single atoms, the one of higher covalence or the transition element is the central atom. Examples are trivalent P over divalent O in $POCl_3$; tetravalent C over trivalent N, and O, in NCO^-; N over O in NOF; and the transition element V over O in $VOCl_3$.
3. For species containing two or more single atoms with equal covalence, the larger atom from a higher-numbered period will be central. An example is $SOCl_2$, where S from the third period is selected rather than O from the second.

There are, however, a few exceptions, such as nitrous oxide, fulminate ion, disulfur monoxide, thiosulfate ion, and sulfur nitrifluoride, where the respective atomic arrangements are NNO, CNO^-, SSO, SSO_3^{2-}, and NSF. Fulminate ion (CNO^-) is the only known isomer of inorganic origin for a more stable counterpart, namely, the cyanate ion (NCO^-). Disulfur monoxide (S_2O) and thiosulfate ion ($S_2O_3^{2-}$), on the other hand, can be seen as derived after replacing an O from each OSO and SO_4^{2-} with S.

Recall also that H and F always take up the peripheral position in any polyatomic molecules and ions.

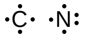
To illustrate the direct electron-pairing approach in writing Lewis structures, examples from diatomic molecules and ions are shown first, followed by polyatomic species.

Diatomic Covalent Species

Diatomic molecules and ions obviously represent a small portion of all covalent species. To write Lewis structures for these species,

1. Write Lewis symbols for the two neutral atoms. For neutral molecules, proceed to step 3.
2. For each negatively/positively charged ion, add/remove an electron to/from an atom to produce Lewis symbols with equal numbers of unpaired electrons.
3. Pair all unpaired electrons to give covalent bond(s). The already paired electrons and atomic charges will automatically become lone pair(s) and formal charges.

Writing Lewis structures for diatomic species is illustrated by CN^-, NO^+ and CO. According to step 1, Lewis symbols for neutral atoms are,



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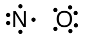

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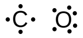

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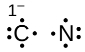
Because CN^- has a single negative charge, an electron is added to the C of **1** to give **4**, both with the same number of unpaired electrons (step 2). Carbon in **4** therefore has a charge of 1−. An electron is removed from any of two electron pairs on O in **2**, because NO^+ has a single positive charge, to give **5**. Oxygen in **5** has a charge of 1+. No electron is added/removed to/from arrangement **3**, since CO is a neutral species.



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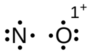

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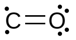

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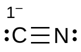
Electron pairing in arrangements **4** and **5** (step 3) results in Lewis structure **7** for cyanide ion and **8** for nitrosonium ion. Each atom in these species has an octet. Nitrogen in structures **7** and **8** has no formal charge and it is not shown explicitly. Carbon in **6** would have a suboctet (6 electrons) after two unpaired electrons in **3** are paired to form a C=O double bond. This violates the octet rule. Carbon in **6** can achieve an octet after a lone pair on O is converted to a π bond to give Lewis structure **9**. Formal charge for the O/C increases by one unit more positive/negative. It should be stressed that carbon monoxide is the only exception to the procedure.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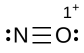
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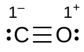
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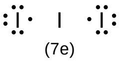
Polyatomic Covalent Species

Most covalent species are polyatomic. They can have two types of peripheral atoms: monovalent (H, F, Cl, Br, and I) as in H_2O, SF_4, I_3^-, or ClF_6^+; polyvalent (O, S, and N) as in SO_2, SO_3, SOF_4, PO_4^{3-}, SO_3^{2-}, SO_4^{2-}, N_2O, or N_3^-. To write Lewis structures for polyatomic molecules and ions,

1. Write Lewis symbols for surrounding atoms around the central atom so that the unpaired electrons of the former face the latter. (The number of valence electrons on the central atom is given in a small bracket below its symbol as a reminder.)
2. For a polyatomic anion with monovalent surrounding atoms, add an electron to the central atom for each negative charge. For a polyatomic anion with at least one polyvalent surrounding atom, add one electron for each unit of charge to surrounding polyvalent atoms one after another. For any polyatomic cation, remove an electron from the central atom for each positive charge. A new number of electrons and charge now appears on each atom.
3. Sum the number of unpaired electrons on surrounding atoms. The same number of electrons from the central atom is needed for pairing to yield bonds. The remaining electrons on the central atom will form lone pair(s). In this so-called parent structure, the central atom may have an octet, less than an octet, or more than an octet of electrons. A parent structure with monovalent peripheral atoms, or with a less than an octet on the central atom, or with an octet that is not allylic/propargylic/allenic[1] represents a single Lewis structure. A parent structure in which the central atom has more than an octet and there is at least one polyvalent peripheral atom (O/S/N) must be reduced to an octet, or, if that is not possible, to a lower, all single-bonded structure. This is done by converting sufficient or all π bond(s) to lone pair(s) on the peripheral atom (O/S/N). Formal charge on the central atom increases by one unit more positive for each conversion. Formal charge on a peripheral atom (O/S/N) becomes one unit more negative for each conversion.
4. A full octet structure that is allylic/propargylic/allenic, either the parent structure or one derived from it, can be converted to multiple resonance structures. This is done by changing a π bond to a lone pair on one peripheral atom at the same time that a lone pair on another peripheral atom is converted to a π bond. Formal charges change accordingly.

As an illustration, consider three polyatomic covalent species: I_3^-, SO_3^{2-}, and N_2O.

EXAMPLE 1: I_3^-. According to step 1, Lewis symbols of terminal atoms are written next to a middle I that carries 7 valence electrons (arrangement 10).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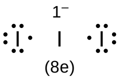
Since I_3^- has a negative charge, and to comply with step 2 for monovalent peripheral atoms, an electron is added to central I in **10**. Now, it has 8 electrons and a 1− charge as in arrangement **11**.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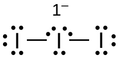
Addition of an electron to either terminal I in **10** cannot be done because the only unpaired electron on it is needed for pairing to form a single bond. (Similarly, removing an electron from a monovalent surrounding atom in a polyatomic cation should not be done, because it will produce two unpaired electrons, thus promoting the formation of a double bond. All five monovalent H, F, Cl, Br, and I are known to form only single bonds with a central atom.) Moving next to step 3, two unpaired electrons on terminal atoms in **11** can be paired to give two I^-–I single bonds. The remaining 6 electrons on the central atom in **11** form three lone pairs to produce Lewis structure **12**.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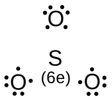
EXAMPLE 2: SO_3^{2-}. Three O's each carrying 2 unpaired electrons are placed around S with 6 electrons (arrangement **13**).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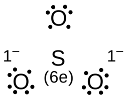
Since SO_3^{2-} has a double negative charge, two electrons are then added to any two outer atoms in **13**. The number of unpaired electrons on each of these two O atoms becomes one and the charge becomes 1− as in **14** (step 2).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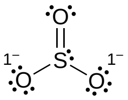
Four unpaired electrons from outer O's in **14** can be paired to give the parent structure **15**. The central S in **15** has a lone pair and four bonds (10 electrons).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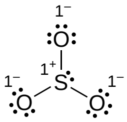
On the basis of agreement between measured bond lengths/orders and experimental values, Suidan et al. (*17*) and Straub (*18*) concluded that for nonmetal oxymolecules and oxyanions with central atom X from period 3 and above in groups IV–VII and "0", the X(1+)–O(1−) single-bonded structures that follow the octet rule are closer to reality than the X=O double-bonded parent structures. Here, the octet is achieved by converting sufficient π bonds to lone pairs toward O's and adjusting formal charges accordingly. Structure **15**, for instance, can be modified in this manner to structure **16**. Its central S contains three single bonds and a lone pair (formal charge 1+). The sum of the formal charges in **16** equals the charge for the ion.



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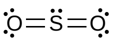
By a similar approach, covalent ions such as PO_4^{3-} and SO_4^{2-} each give one structure instead of four and six resonance structures, respectively, as suggested by some general chemistry textbooks. On the other hand, SO_2 gives two resonance structures and SO_3 gives three, instead of one. If we apply the proposed procedure for SO_2, it will end up with parent structure **17**, where the central S is in the state of 10 electrons (steps 1–3). It becomes an octet after a π bond in **17** is converted to a lone pair towards O to give **18** (step 3). The second resonance structure for SO_2 (**19**) is deduced from the first allylic structure **18** (step 4), as shown below. Covalent species such as SOF_4 produce a parent structure with 12 electrons on S: a double S=O and four single S–F bonds (no lone pair). Conversion of the only double bond to a single bond yields an all-single-bonded structure with 10 electrons on S. Any of the completely single-bonded (octet or expanded octet) structures derived from a higher expanded-octet parent structure is a Lewis structure for the species.



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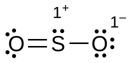

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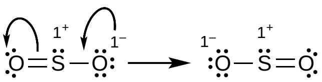
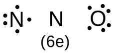


(18) **19**

Example 3: N_2O. The middle N carrying 5 electrons is written between N and O, which have three and two unpaired electrons, respectively (arrangement **20**). Pairing of 5 unpaired electrons from terminal atoms in **20** will give parent structure **21**. The middle N here is in the state of 10 electrons. It can be reduced to 8 by converting a π bond of the triple N≡N in **21** to a lone pair towards the outer N, yielding **22**. An allenic **22** can be used to produce the propargylic resonance structures **23** and **24** as shown below. Three resonance structures representing nitrous oxide (**22**, **23**, and **24**) can be interconverted in a similar fashion from any selected structure.



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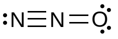

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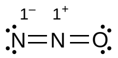

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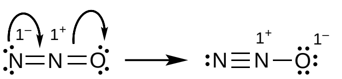
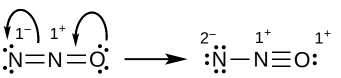


(22) **23**



(22) **24**

Other Covalent Species

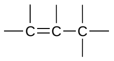
It is possible to utilize the method of writing Lewis structures described above for covalent species containing transition elements in their maximum oxidation states (d^0) as central atoms—for example, $VOCl_3$, CrO_3, CrO_2Cl_2, CrO_4^{2-}, and MnO_4^-. This method can also be applied to polyatomic molecules and ions with more than a single layer of surrounding atoms, such as HSO_4^-, H_2SO_4, HONO, HNO_3, H_2CrO_4, $HMnO_4$, and $HClO_4$; covalent species without clearly defined central atoms, such as H_2O_2, N_2F_2, NH_2OH; and the whole range of organic molecules.

Conclusion

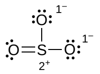
We hope that the direct electron pairing in writing Lewis structures as elaborated in this article will provide a student-friendly approach to this important but confusing topic. It involves the pairing of all unpaired electrons on surrounding Lewis symbols to yield a single parent structure. Resonance structures are multiple Lewis structures produced from an octet and allylic/propargylic/allenic parent structure or its derivative. An important advantage of this approach is the lack of need to calculate formal charges, which are obtained almost automatically when an electron is added to or removed from an atom or when a π bond is converted to a lone pair and vice versa. Once students are familiar with the derivation of some Lewis structures on paper, they are in a position to produce structures for most covalent species.

Note

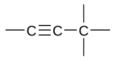
1. Here we define allylic, a term referring to the moiety



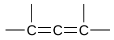
as a structure having moieties like 18/19 or



Propargylic, which is associated with the moiety



refers to a structure with a moiety such as 23/24. Allenic, which designates the moiety



is defined as a structure having a moiety like 22. In each case, the outlying single bonds from the former are replaced by lone pairs to give the latter.

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