

Learning Guide Module

Subject Code: Chem 1 General Inorganic Chemistry

Module Code: 4.0 Chemical Bonding

Lesson Code: 4.5 **Resonance** Time Frame: **30 minutes**

Components	Task	TA ¹	TA^2
		(min)	(min)
Target	After completing this module, you are expected to:	0.5	
	1. draw the resonance structures of		
	molecules and ions.		
	2. apply the concept of resonance to		
	explain the chemical behavior of		
	some molecules/ ions. 3. apply formal charge to resonance structures.		
***	3. appry formal charge to resonance structures.	1.7	
Hook		1.5	
	Blue horse Red donkey		
	Purple mule Figure 1.0 A Purple Mule, Not a Blue Horse and a Red Donkey (Siverberg, 2013, p. 307)		
	Mule is a blend of a horse and donkey (Jones and Atkins, 2000 p.		
	337). A mule is a genetic mix, a hybrid, of a horse and a donkey: it is		
	not a horse one instant and a donkey the next. This genetic mix is		
	related to our topic in this module, which is resonance.		
Ignite	The Concept of Resonance	16	
	The Need for Resonance Structures To understand this issue, consider ozone (O ₃), an air pollutant at ground level but an absorber of harmful ultraviolet (UV) radiation in the stratosphere. (Silberberg, 2013, p. 306) There are two Lewis structures that can be written for ozone.		

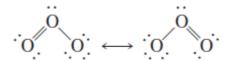






In structure I, oxygen B has a double bond to oxygen A and a single bond to oxygen C. In structure II, the single and double bonds are reversed. You can rotate I to get II, so these are *not* different types of ozone molecules, but different Lewis structures for the *same* molecule. (Silberberg, 2013, p. 306)

We would expect that O-O bond in O₃ to be longer than the O=O bond because double bonds are known to be shorter than single bonds. Yet experimental evidence shows that both oxygen-to-oxygen bonds are equal in length(128 pm). We resolve this discrepancy by using *both* Lewis structures to represent the ozone molecule:



Each of these structures is a resonance structure. A **resonance structure**, then, is one of two or more Lewis structures for a single molecule that cannot be represented accurately by only one Lewis structure. The double-headed arrow(\leftrightarrow) indicates that the structures shown are resonance structures (Chang and Overby, 2011,p.303). The situation in which two or more plausible Lewis structures contribute to the "correct" structure is called **resonance**. The true structure is a resonance hybrid of plausible contributing structures. (Petrucci et. al.,2017,p 432)

Resonance structures are not real bonding depictions: O₃ does not change back and forth quickly from structure I to structure II. The actual molecule is a **resonance hybrid**, anaverage of the resonance forms.(Silberberg,2013,p.306)

A common misconception about resonance is the notion that a molecule such as ozone somehow shifts quickly back and forth from one resonance structure to the other. Keep in mind that *neither* resonance structure adequately represents the actual molecule, which has its own unique stable structure. "Resonance" is a human invention designed to address the limitations in these simple bonding models. (Chang and Overby,2011,p 303-304)

Electron Delocalization Our need for more than one Lewis structure to depict O_3 is due to **electron-pair delocalization**. In a single, double, or triple bond, each electron pair is *localized* between the bonded atoms. In a resonance hybrid, two of the electron pairs (one bonding and one lone pair) are *delocalized*: their density is "spread" over few adjacent atoms.

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In O_3 , the result is two identical bonds, each consisting of a single bond (the localized pair) and a *partial bond* (the contribution from one of the delocalized pairs). We draw the resonance hybrid with a curved dashed line to show the delocalized pair:

(Silberberg, 2013, p. 307)

Resonance is very common. For example, benzene (C_6H_6) has two important resonance forms in which alternating single and double bonds have different positions. The actual molecule is an average of the two forms with six C-C bonds and three electron pairs delocalized over all six C atoms. The delocalized pairs are often shown as a dashed circle (or sometimes simply a circle):

resonance forms

or

resonance hybrid

or

$$\bigcirc \bigcirc \bigcirc \bigcirc \bigcirc$$
 or $\bigcirc \bigcirc$

(Silberberg, 203, p.307)

The shorthand notation reminds us that benzene is a blend of two resonance structures – it emphasizes that the C=C double bonds cannot be assigned to specific edges of the hexagon. Chemists use



both representations of benzene interchangeably. (Brown t. al.,2012, p.312)

Resonance stabilizes a molecule by lowering its total energy. This stabilization, which can be explained only by quantum mechanics, makes benzene *less reactive* than expected for a molecule with three carbon-carbon double bonds.(Atkins & jones, p 339)Resonace results in the greatest lowering of energy when contributing structures have equal energies. (Jones and Atkins, 2000, p 339)

Example 1. Draw resonance structures for the nitrate ion, NO₃-.

Solution: Follow the step by step procedure in writing Lewis structures.

(Zumdhal and Zumdhal, 2012, p. 177)

There are three resonance structures for the nitrate ion. They simply show that the actual structure is an average of the three resonance structures. Resonance is necessary to compensate for the defective assumption of the localized electron model. Do not forget to enclose the Lewis structure in a bracket and write the negative charge on the upper right hand corner.

Formal Charge: Selecting the More Important Resonance Structure

If one resonance form "looks" more like the resonance hybrid than the others, it "weights" the average in its favor. One way to select the more important resonance form is by determining each atom's **formal charge**, the charge it woud have *if the bonding electrons were shared equally*.(Silberberg,2013,p. 308)

Formal Charge(FC) = (number of valence electrons in an uncombined atom) – (number of valence electrons assigned to the bound atom in a Lewis structure) (Hill et al.,2005, p 357)

- Count *lone-pair electrons* as belonging entirely to the atom on which they are found.
- <u>Divide bond-pair electrons</u> equally between the bonded atoms.

(Petrucci et. al., 2017,p.428)

The following are general rules that can help to determine the plausibility of a Lewis structure based on its formal charges.

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- The sum of the formal charges in a Lewis structure must equal zero for a molecule and must equal the magnitude of the charge for a polyatomic ion.
- Where formal charges are required, they should be as small as possible.
- Negative formal charges usually appear on the <u>most</u> electronegative atoms; positive formal charges, on the *least* electronegative atoms.
- Structures having formal charges of the *same* sign on adjacent atoms are *unlikely*.

(Petrucci et. al.,2017, p.428)

Let us now apply the concept of formal charge to the ozone molecule.

Valence
$$e^-$$
 6 6 6 e^- assigned to atom 6 5 7

$$\begin{array}{c}
\text{Difference} \\
\text{(formal charge)}
\end{array} 0 + 1 - 1$$

(Chang and Overby, 2011, p.301)

(Petrucci et al, 2017, p.432)

Since it is a molecule, the sum of all the charges is zero.

Example 2. Draw resonance structures for the carbonate ion, CO₃²⁻. Indicate formal charges.

Solution: Follow the step by step procedure in writing Lewis structures

$$\begin{vmatrix} : \circ \cdot^{0} & : \ddot{\circ} :^{-1} & : \ddot{\circ} :^{-1} \\ -1 : \ddot{\circ} - C - \ddot{\circ} :^{-1} \longleftrightarrow \overset{0 \dots}{\circ} = C - \ddot{\circ} :^{-1} \longleftrightarrow \overset{-1}{\circ} : \ddot{\circ} - C = \ddot{\circ} \end{vmatrix}^{2}$$

The sum of the formal charges is equal to -2(charge of the ion). Based on the concept of formal charge, which is the most important resonance structure?

According to experimental evidence, all carbon-to-carbon bonds

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in O_3^{2-} are equivalent. Therefore, the properties of the carbonate ion
are best explained by considering its resonance structures together.
(Chang and Overby,2011, p.304)

Example 3.Draw three resonance structures for the molecule nitrous oxide, N_2O (the atomic arrangement is NNO). Indicate formal charges. Rank the structures in their relative importance to the overall properties of the molecule.

We follow the procedure for drawing Lewis structure and calculating formal charges.

$$(5-6) (5-4) (6-6) (5-5) (5-4) (6-7) (5-7) (5-4) (6-5)$$

$$: N = N - O : N = O$$

We see that three structures show formal charges. Structure (b) is the most important one because the negative charge is on the more electronegative atom. Structure (c) is the least important on because it has a larger separation of formal charges. Also, the positive charge is on the more electronegative oxygen atom. (Chang and Overby.2011,p.305)

Navigate

PART I. NONGRADED ASSESSMENT



(For students practice only)

- 1. Show all resonance structures for the following:
- a. NO_2^-
- b. SCN⁻ (C is the central atom)
- c. OCN⁻ (C is the central atom)
- d. N_2O_4 (N_2O_4 exists as O_2N-NO_2 .)

PART II GRADED ASSESSMENT

Teachers prerogative: Teachers can choose problems 4-5 as an additional graded assessment if you find that students needs additional assessment to evaluate their understanding.

- 1. Draw all resonance structures of SO₃ molecule. Indicate formal charges. Are all structures equivalent?
- 2. Through appropriate Lewis structures, show that the phenomenon of resonance is involved in nitrite ion. Include formal charges.
- 3. Write two equivalents resonance structures for the bicarbonate ion, HOCO₂. Draw the resulting resonance hybrid structure for the bicarbonate ion. (Hill, et. al., 2005, p. 381)

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Knot	Summary:	2	
	 "Resonance" is a human invention, designed to address the limitations of simple bonding models. (Chang, 2005,p. 366) Resonance – Often, more than one plausible Lewis structure can be written for a species; this situation is called resonance. In these cases the true structure is resonance hybrid of two or more contributing structures. (Petrucci et al,2017, p.454) Formal charge is the electric charge difference between the valence electrons in an isolated atom and the number of electrons assigned to that atom in a Lewis structure. (Chang and Overby, 2011,p.300) 		

¹Time allocation suggested by the teacher

Answer to the practice exercises

a.
$$\frac{NO_2^{-} \quad \left[\stackrel{\dots}{\circ} = \stackrel{\dots}{N} - \stackrel{\dots}{\circ} : \right]^{-} \longleftrightarrow \left[\stackrel{\dots}{\circ} \stackrel{\dots}{\circ} - \stackrel{\dots}{N} = \stackrel{\dots}{\circ} \right]^{-}}{SCN^{-} \quad \left[: \stackrel{\dots}{S} - C = N : \right]^{-} \longleftrightarrow \left[: \stackrel{\dots}{S} = C = \stackrel{\dots}{N} : \right]^{-} \longleftrightarrow \left[: S = C - \stackrel{\dots}{N} : \right]^{-}}$$
b.

$$\begin{array}{c} \text{OCN}^{-} & \vdots & \vdots & \cdots & \vdots \\ \vdots & \vdots & \cdots & \vdots \\ \text{CC} & \vdots & \vdots \\ \text{CC} & \vdots & \vdots \\ \text{CC} & \vdots \\ \text{CC}$$

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²Actual time spent by the student(for information purposes only



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