

Chemistry 51

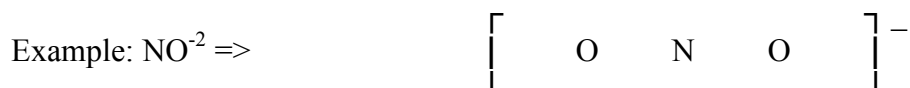
Experiment 5

Introduction to Molecular Modeling

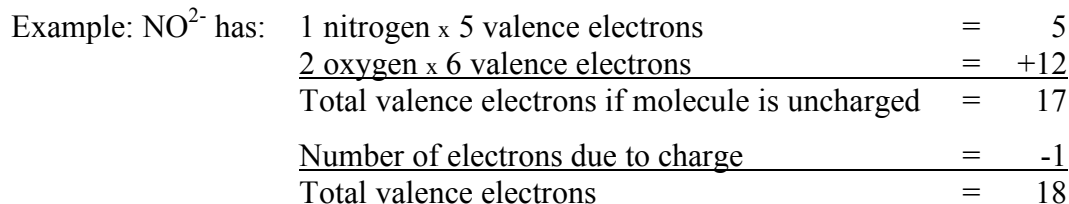
RULES FOR CONSTRUCTING LEWIS DOT FORMULAS

In order to determine the three-dimensional geometry of a molecule, a correctly constructed dot structure should first be drawn. The following rules can be followed in order to construct a correct Lewis dot structure. As an example, NO^{2-} will be used.

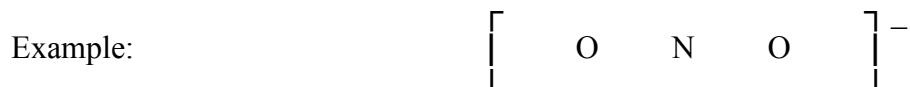
1. Draw a skeleton structure by placing outer atoms around the central atom. Include the charge if the molecule is an ion.



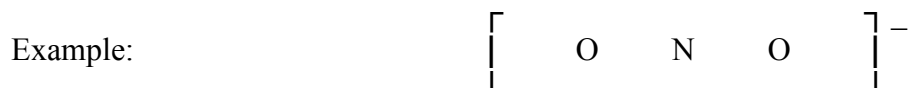
2. Add up the number of valence electrons contributed by each of the atoms in the molecule or ion. If the molecule is negatively charged, add one electron for each negative charge. If the molecule is positively charged, subtract one electron for each positive charge.



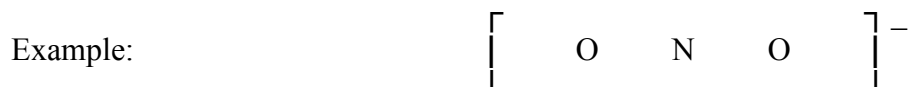
3. Distribute one pair of electrons between the central atom and each of outer atoms first.



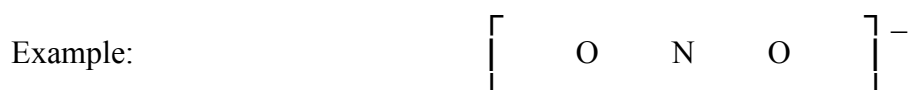
4. Distribute the remaining electrons, in pairs, around the outer atoms so that each outer atom has eight electrons (except for hydrogen).



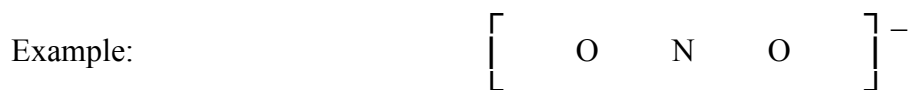
5. If there are still electrons that need to be placed in the dot structure, as is the case with our example, place those electrons around the central atom.



6. Count the number of electrons around each atom. If the central atom has fewer than eight electrons, move a pair or two pairs of electrons from an outer atom to be shared between the outer atom and the central atom in order for the central atom to have eight electrons around it.



Nitrogen only has 6 electrons around it. A double bond is formed between one of the oxygen atoms and the nitrogen. Now our dot structure is complete.



MOLECULAR STRUCTURE LABORATORY - PROCEDURE

For each of the compounds or polyatomic ions numbered 1 through 12 on the following pages, complete the steps below. There are examples worked out for you following these steps so you know what is expected.

1. Calculate the electronegativity difference between bonding atoms and predict the kind of bonding present (*i.e.*, ionic bonding, polar covalent bonding, or non-polar covalent bonding).
2. State whether it is a true molecule or whether a crystal lattice (a 3-dimensional checkerboard) is present. If the bonding is polar covalent or non-polar covalent it is molecular. If the bonding is ionic, no molecule is formed and a crystal lattice is present which you will not be required to draw. If it is ionic, simply write "crystal lattice" for step 2 and go on to the next compound or ion.
3. If it is a true molecule, draw the Lewis dot structure for the molecule. Rules for drawing dot structures are on the first page of this experiment.
4. Only if there is a true molecule, build (then draw) the molecule using the ball, stick and spring model set. Use yellow balls for hydrogen, black balls for carbon, red balls for oxygen and green balls for halogens. Use sticks for single bonds and springs for multiple bonds (two springs for double bonds and three springs for triple bonds).
5. View your model and then give the electronic shape of the molecule. Choose from:

linear	trigonal planar	tetrahedral
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6. After determining the electronic shape, predict the molecular shape. Choose from:

linear	bent	trigonal planar	trigonal pyramid	tetrahedral
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7. Give the bond angles involved if there are three or more atoms in the molecule.

8. State whether the molecule is polar or non-polar. Polar requires a) polar bonds and b) a region of the molecule which is partially positively charged and a region of the molecule which is partially negatively charged. This is caused by an uneven distribution of electron density about the molecule. If the molecule is polar then indicate the partial negative (δ^-) and partial positive (δ^+) regions in your drawing.

MOLECULAR STRUCTURE LABORATORY - EXAMPLES

- NaCl
1. $3.0 - 0.9 = 2.1$ therefore ionic bonding
 2. crystal lattice present
 3. Structure need not be drawn

- H₂O
1. $3.5 - 2.1 = 1.4$ polar covalent bonding
 2. true molecule
 3. H—O—H
 4. Model has 2 yellow balls and one red ball and 2 sticks (two sticks are for the single bonds between the oxygen and hydrogen.)
 5. Electronic geometry is tetrahedral
 6. Molecule has a bent or angular geometry
 7. Bond angles are approximately 109.5°
 8. Molecule is polar

- CH₂Cl₂
1. 3.0 highest electronegativity
 -2.1 lowest electronegativity
 0.9 polar covalent bonding
 2. true molecule
 3.

$\begin{array}{c} \text{Cl} \\ \\ \text{H} - \text{C} - \text{H} \\ \\ \text{Cl} \end{array}$	or	$\begin{array}{c} \text{H} \\ \\ \text{H} - \text{C} - \text{Cl} \\ \\ \text{Cl} \end{array}$
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 4. Model has 4 sticks, 2 yellow balls, 2 black balls & 2 green balls
 5. Electronic Geometry is tetrahedral
 6. Molecular geometry is tetrahedral
 7. Bond angles are 109.5°
 8. Molecule is polar.

Introduction to Molecular Modeling

Follow the 8 steps to determine the three-dimensional geometry of the molecules, ions or ionic compounds below. Draw a picture of the molecule if you can.

1. Cl_2

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

2. HF

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

3. KCl

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

4. BaO

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

5. CO_3^-

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

6. PH_3

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

7. C_2H_6 (Describe the geometry about each central carbon atom)

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

8. CO_2

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

9. H₂S

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

10. CO

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

11. C₂H₄ (Describe the geometry about each central C atom)

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.

12. SiH₄

- 1.
- 2.
- 3.
- 4.
- 5.
- 6.
- 7.
- 8.