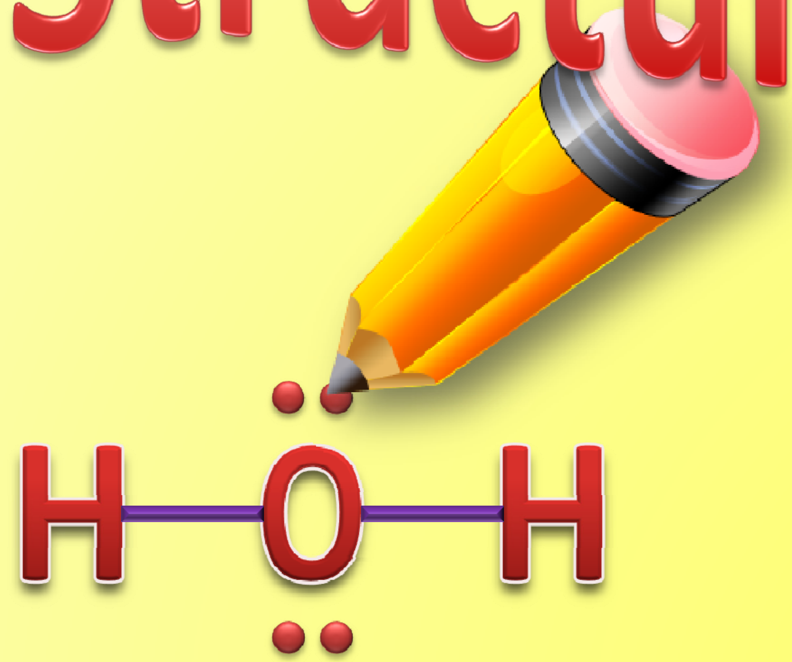
Lewis Structures



Purpose

Lewis structures show how valence electrons are arranged among atoms in a compound using dots to represent the valence electrons that are not shared in a covalent bond.

Drawing Lewis Structures

(for elements in periods 1 and 2)

Procedure

- Sum the valence electrons.
- Use a pair of electrons to form each bond (shown with a connecting line).
  - Called *bonding electrons*.
- Arrange the remaining electrons to satisfy the duet rule for hydrogen and the octet rule for other elements (drawn as dots).
  - Called *lone pairs*.

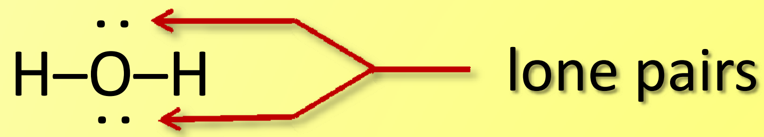
Drawing Lewis Structures Continued

(for elements in periods 1 and 2)

WRITE DOWN

Example: H_2O

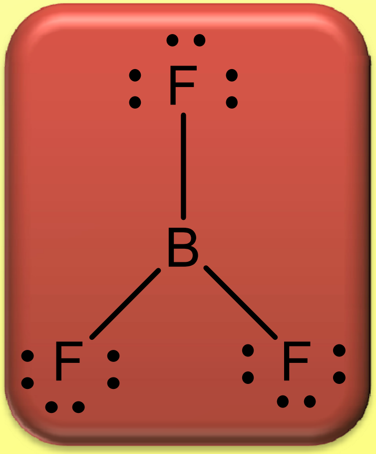
- **<u>Step 1</u>**: Sum the valence electrons.
  - H =1, O = 6;   1 + 1 + 6 = 8
- **<u>Step 2</u>**: Use a pair of electrons per bond (each represented as a line).
  - H–O–H
- **<u>Step 3</u>**: Distribute the remaining electrons (as dots).

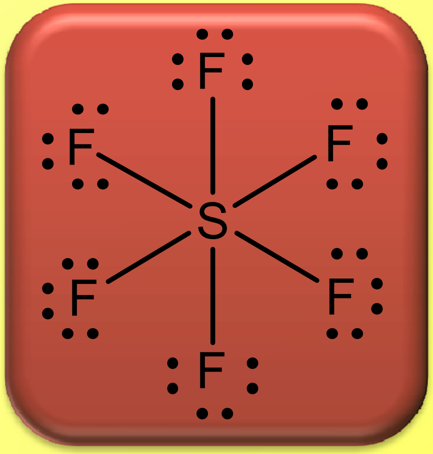


- **<u>Step 4</u>**: Check to see that the duet rule is satisfied for hydrogen and the octet rule is satisfied for all other atoms.

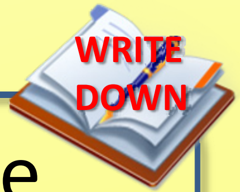
Exceptions to the Octet Rule

- Boron and beryllium tend to form compounds that are electron deficient.
- Elements in period 3 and beyond sometimes exceed the octet rule by using space in *d* orbitals to accommodate extra electrons.
  - In SF_6, for example, S exceeds the octet rule.

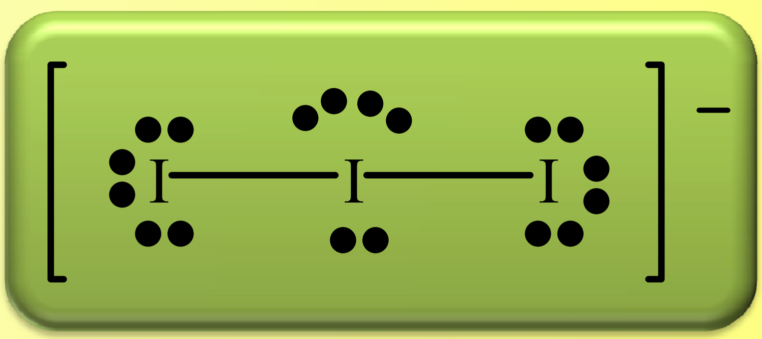




Dealing with Exceptions

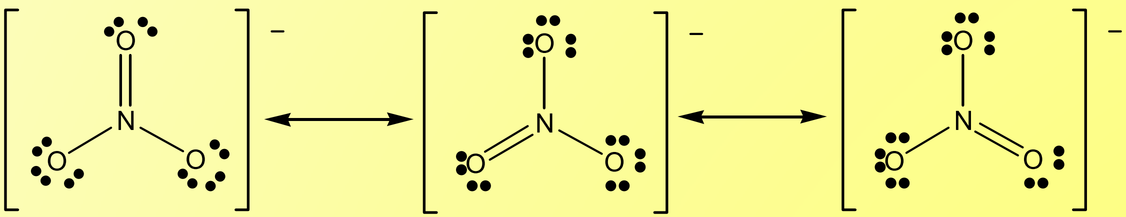


- When writing Lewis structures, satisfy the octet rule first.
- If extra electrons remain, place them on elements having available *d* orbitals.
- If one of several elements exceed the octet rule, assume the electrons are on the central atom.



Resonance

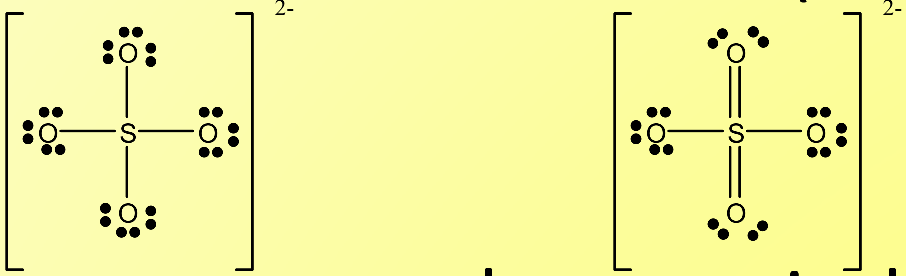
- There may several valid *equivalent* Lewis structures for some molecules.
  - This is called **resonance**.
- The resonance structures for the polyatomic ion NO^{3-} are pictured below.



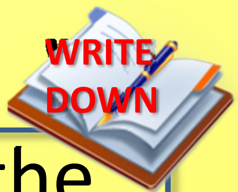
  - The ion does NOT have one double and two single bonds nor does it flip from one to the other structure as it appears.
  - It has 3 equivalent bonds.
  - Resonance is represented by showing the possible Lewis structures with a double headed arrow indicating the actual structure is an average of the resonance structures.

Nonequivalent Lewis Structures

- Sometimes, it is possible to draw different Lewis structures for a molecule (or ion).



- When there are several nonequivalent Lewis structures for a molecule, it is possible to choose among them using formal charge.



- Formal charge is the difference between the number of valence electrons on the free atom and the number of valence electrons assigned to the atom in the molecule.

Formal Charge

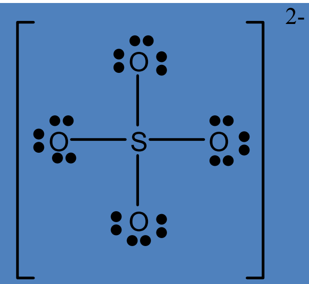
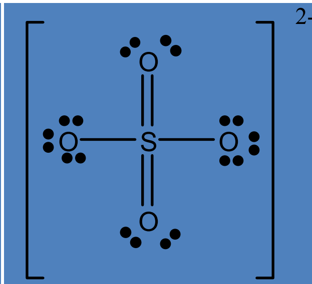
Calculating Formal Charge

- Lone pairs belong entirely to the atom in question.
- Shared electrons are divided equally among the sharing atoms.
  - valence electrons assigned = (number of lone pair electrons) + ½(number of shared electrons)
  - Formal Charge = (valence electrons) – (valence electrons assigned)

Evaluating Lewis Structures with Formal Charge

- Atoms in molecules should have formal charges as close to zero as possible.
- Negative formal charges reside with the most electronegative element.

Example: SO_4^{-2}

Structure		 32 Valence electrons	 32 Valence electrons
Formal Charge	Oxygen with single bonds	Valence electrons assigned: $6 + ½ (2) = 7$ Formal charge: $6 – 7 = –1$	Valence electrons assigned: $6 + ½ (2) = 7$ Formal charge: $6 – 7 = –1$
	Oxygen with double bonds	Valence electrons assigned: – – Formal charge: – –	Valence electrons assigned: $4 + ½ (4) = 6$ Formal charge: $6 – 6 = 0$
	Sulfur	Valence electrons assigned: $0 + ½ (8) = 4$ Formal charge: $6 - 4 = 2$	Valence electrons assigned: $0 + ½ (12) = 6$ Formal charge: $6 – 6 = 0$
	Total	$4(–1) + 2 = –2$ ✗	$2(–1) + 2(0) + 0 = –2$ ✓