Writing Lewis Structures

Rules for writing structures

(1) you must know the order in which the atoms are connected

This is normally determined by experiment and is referred to as the *constitution* of a molecule

General rule: the atom with the lowest electron affinity is usually the central atom

Levels of Structure

Elemental Composition

Empirical Formula

Molecular Formula

Constitution

Configuration

Conformation

Rules for writing structures

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This is normally determined by experiment and is referred to as the ***constitution*** of a molecule

Example: hypochlorous acid has the molecular formula HClO. But the atoms are connected in the order of HOCl

Rules for writing structures

(2) Count the number of valence electrons

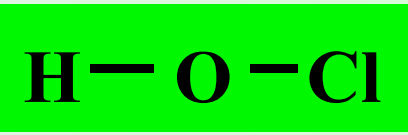
For main group elements this is the same as the group number in the periodic table

Example: hypochlorous acid : HOCl

H	**1 electron**
O	**6 electron**
Cl	**7 electron**
total	**14 valence electrons**

Rules for writing structures

(3) write out the constitution in a form that shows the covalent bonds and count the number of electrons in covalent bonds

Example: hypochlorous acid 

4 electrons in covalent bonds

14 valence electrons

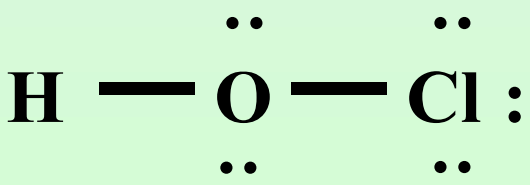
10 electrons remain to be assigned

Rules for writing structures

(4) assign remaining electrons so as to complete the octets of as many atoms as possible.

Example: hypochlorous acid HOCl

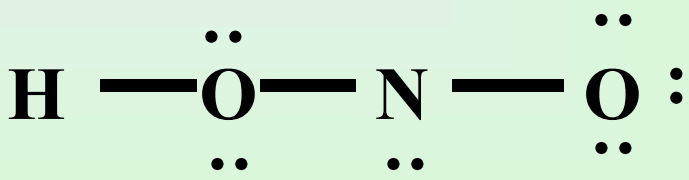
(4 electrons in covalent bonds + 10 more electrons assigned as shown)



Rules for writing structures

(5) when the number of electrons is insufficient to complete the octetes of all of the atoms, assign them to atoms in order of decreasing atom electronegativity.

Example: nitrous acid HNO_2 (HONO)



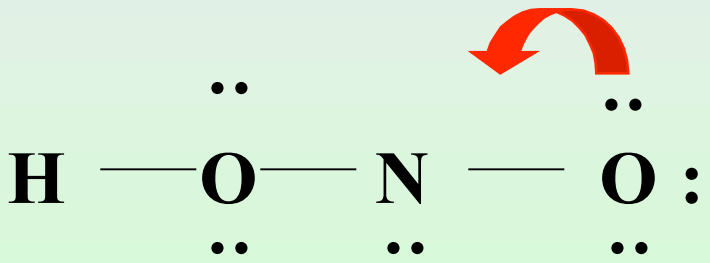
18 valence electrons

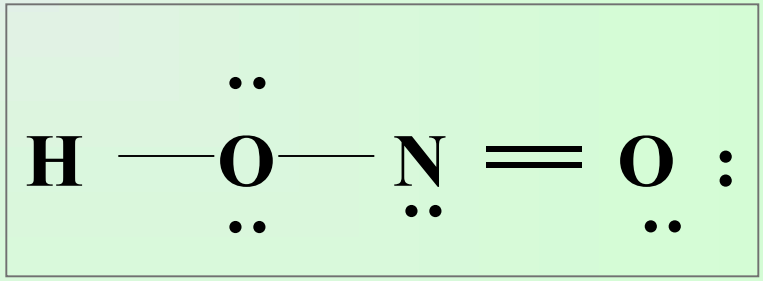
Need to assign 12 electons in addition to 6 found in three bonds

Rules for writing structures

(6) use unshared pairs for double bonds if this will satisfy octet rule.

Example: nitrous acid HONO

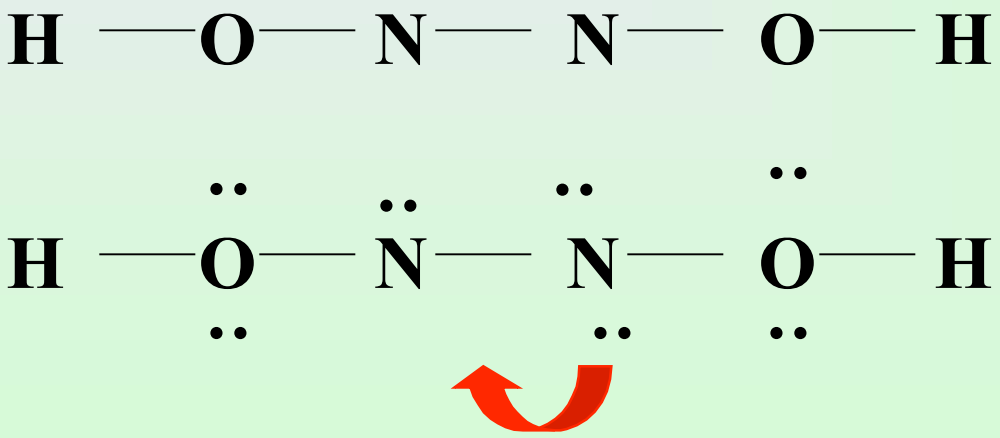




Another example

Example: hyponitrous acid HONNOH

24 valence electrons



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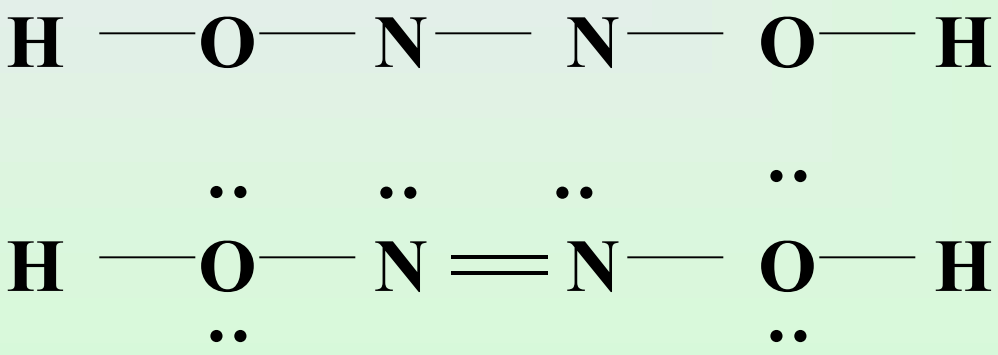
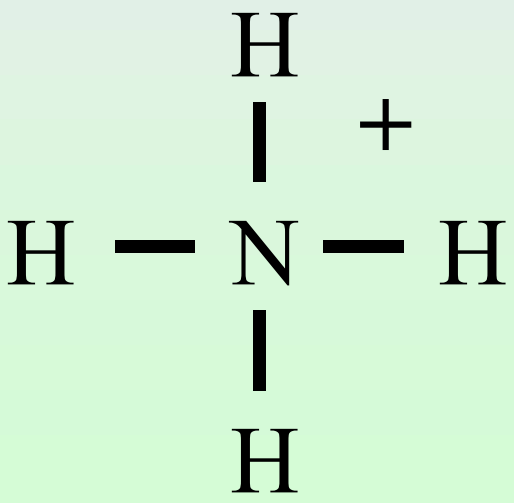


Ions

Subtract one electron for each positive charge

Ammonium ion (NH_4^+)

Number of electrons = 5 + 4 -1 = 8

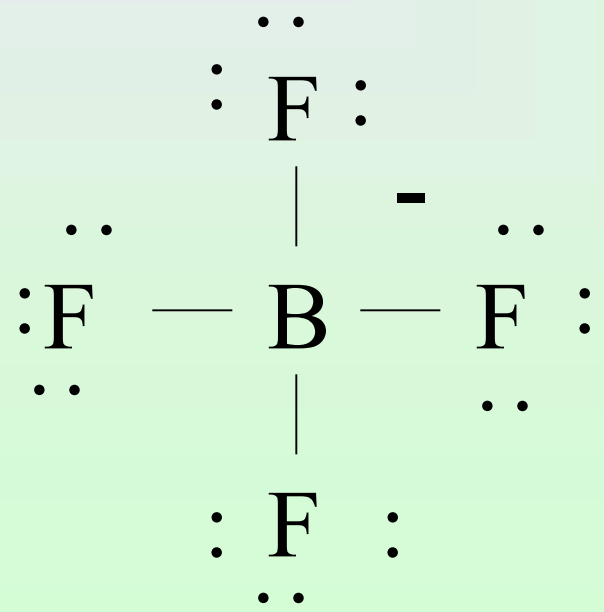


Ions

add one electron for each negative charge

Tetrafluoroborate (BF_4^-)

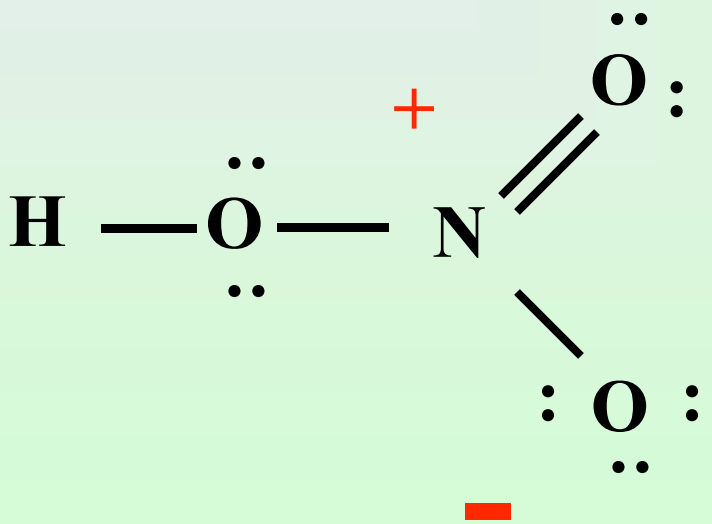
Number of electrons = 3 + 28+1 = 32



Rules for writing structures

(7) assign formal charges

Example : nitric acid HNO_3 $(HONO_2)$



Formal Charge and Lewis Structure

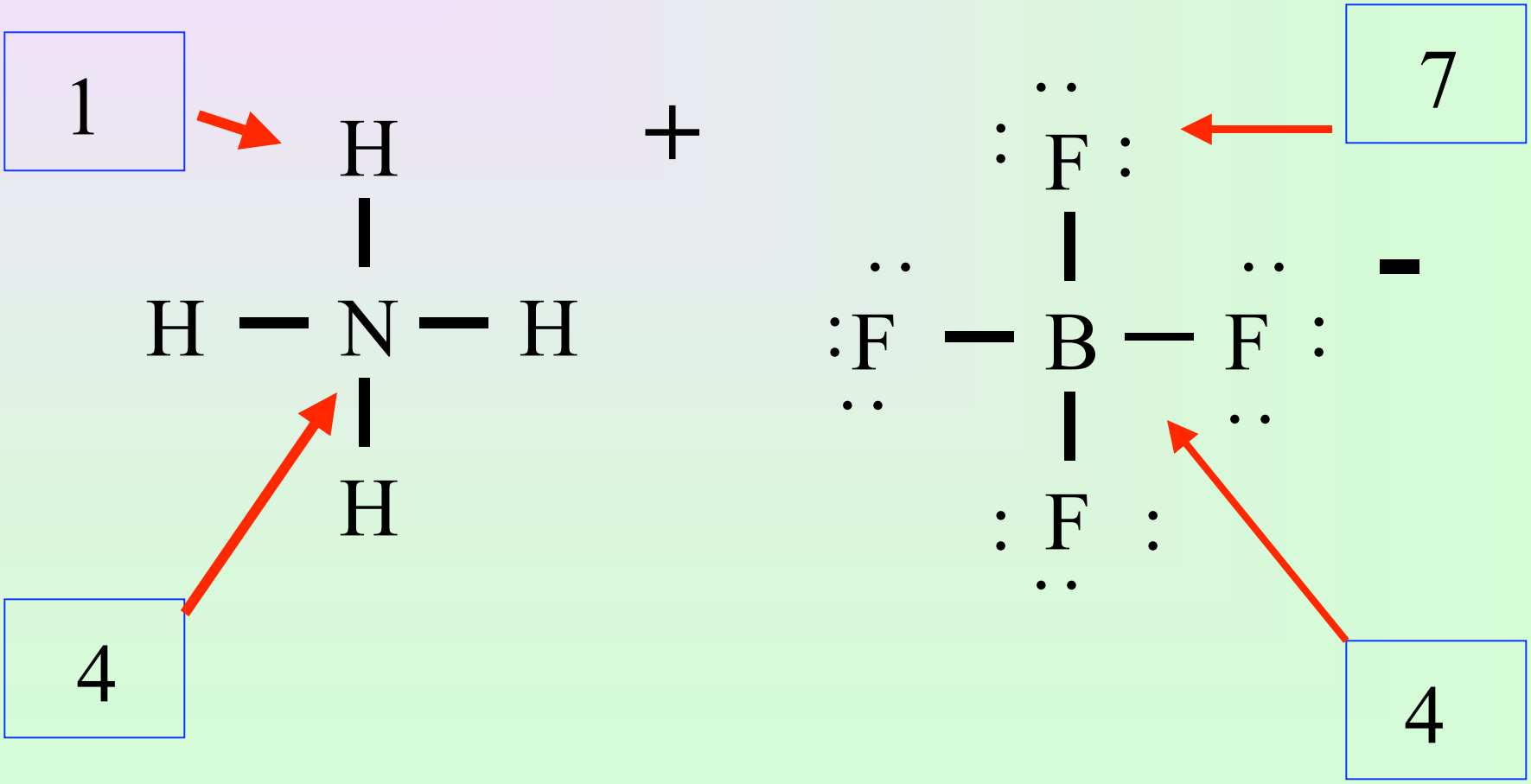
Formal Charge

= number of valence electrons in neutral atom - electron count of atom

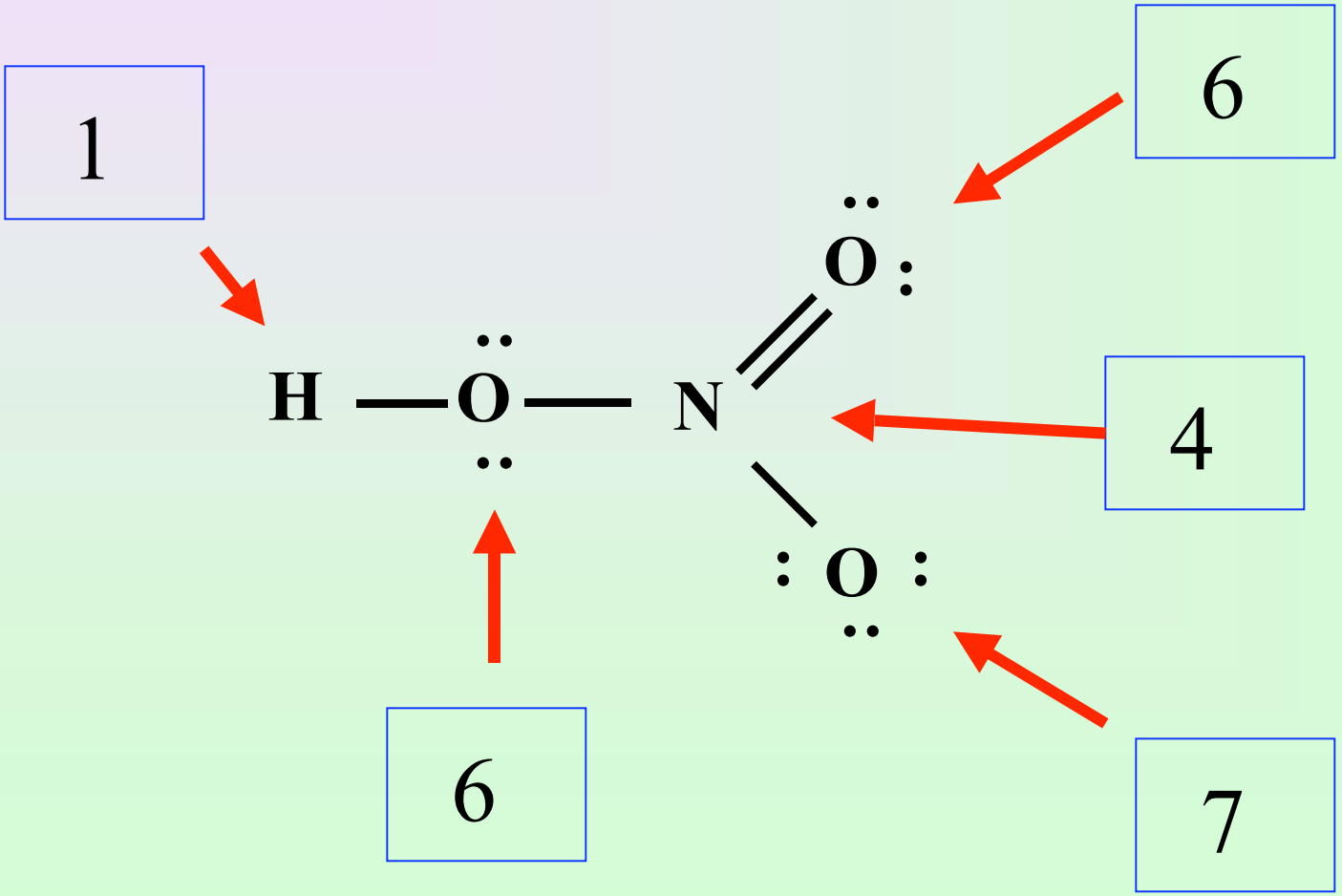
electron count =

number of electrons "owned" by atom + one- half the number of shared electrons

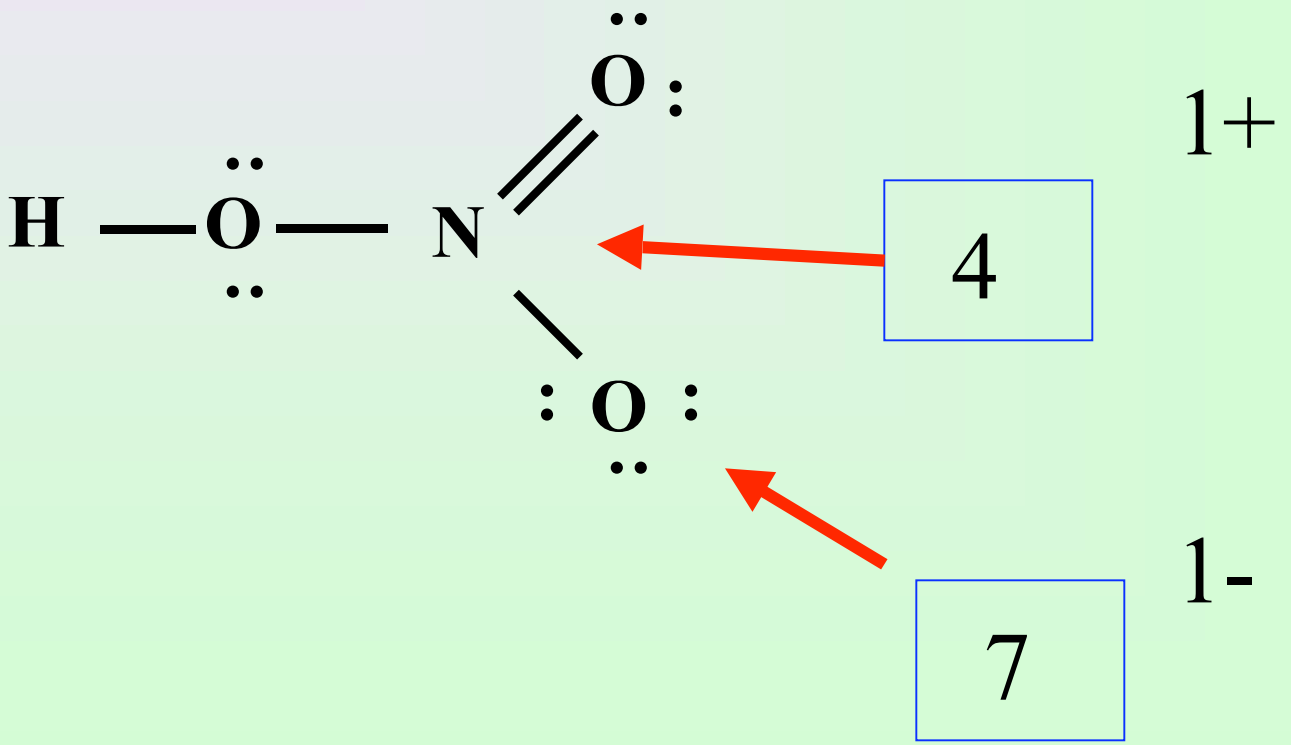
electron counts and formal charges in NH_4^+ and BF_4^-



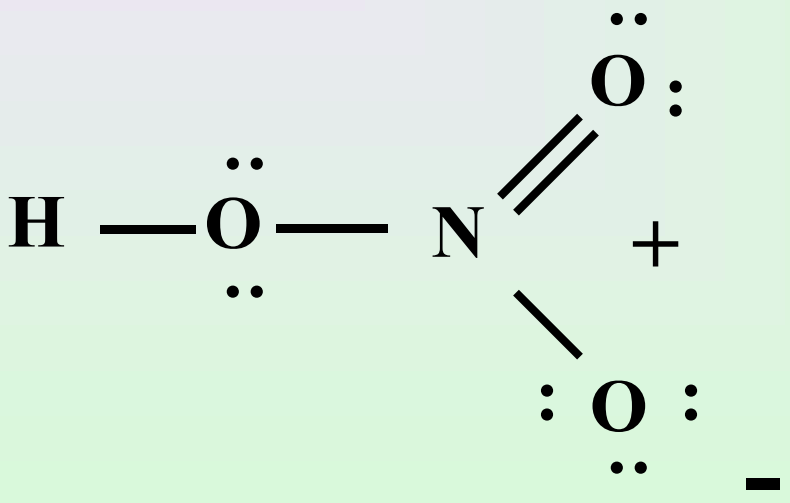
“Electron counts” in nitric acid



Formal charges in nitric acid



Lewis Structure of nitric acid



Formal Charge

does not represent the real charge on an atom in the molecule

it can however be used to determine the validity of a molecules Lewis structure

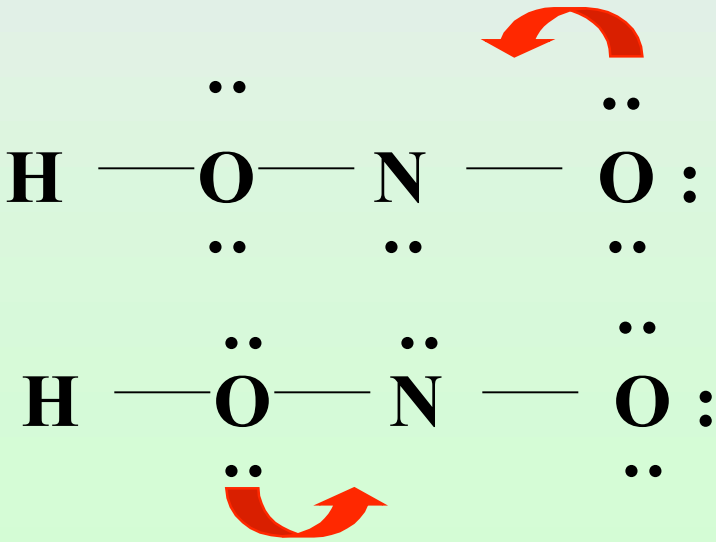
- Try to minimize formal charge in your Lewis structures
- Avoid positive values of formal charge on highly electronegative elements

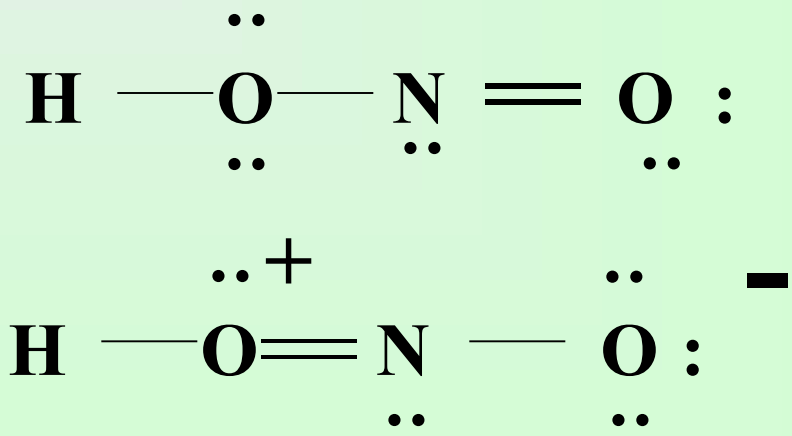
Recall :

Rules for writing Lewis Structures

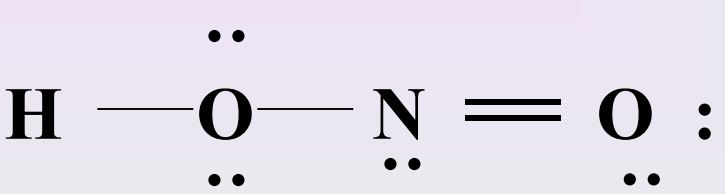
(6) use unshared pairs for double bonds if this will satisfy octet rule.

Example : nitrous acid HONO

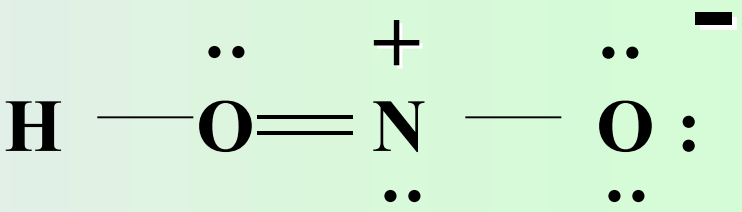




Formal Charge



More stable Lewis Structure



Less stable Lewis Structure

Formal Charge

The sum of the formal charges of all atoms in a given molecule or ion must equal the overall charge on that species

Two Conventions

Oxidation States

Formal Charges

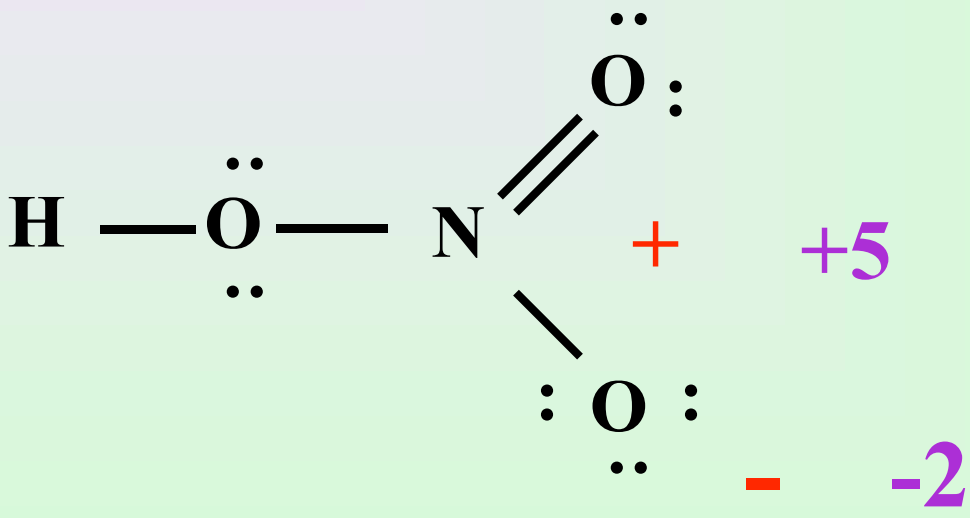
formal charges are closer to actual atomic charges than are oxidation states

but are still only estimations of molecular atomic charge

Lewis Structure of nitric acid

formal charge

oxidation state



oxidation state = electrons lost or gained plus formal charge

The Concept of Resonance

Resonance

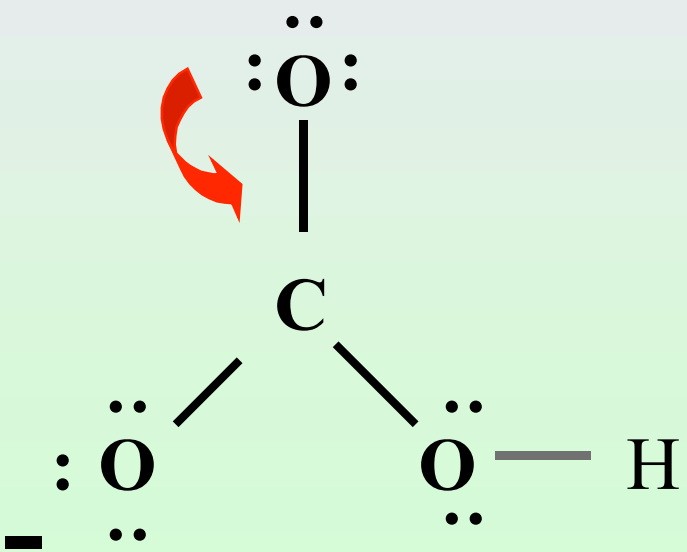
Two or more Lewis structures may be written for certain compounds (or ions)

Recall :

Rules for writing Lewis Structures

(6) use unshared pairs for double bonds if this will satisfy octet rule.

Example :bicarbonate $HOOCO^-$



Recall :

Rules for writing Lewis Structures

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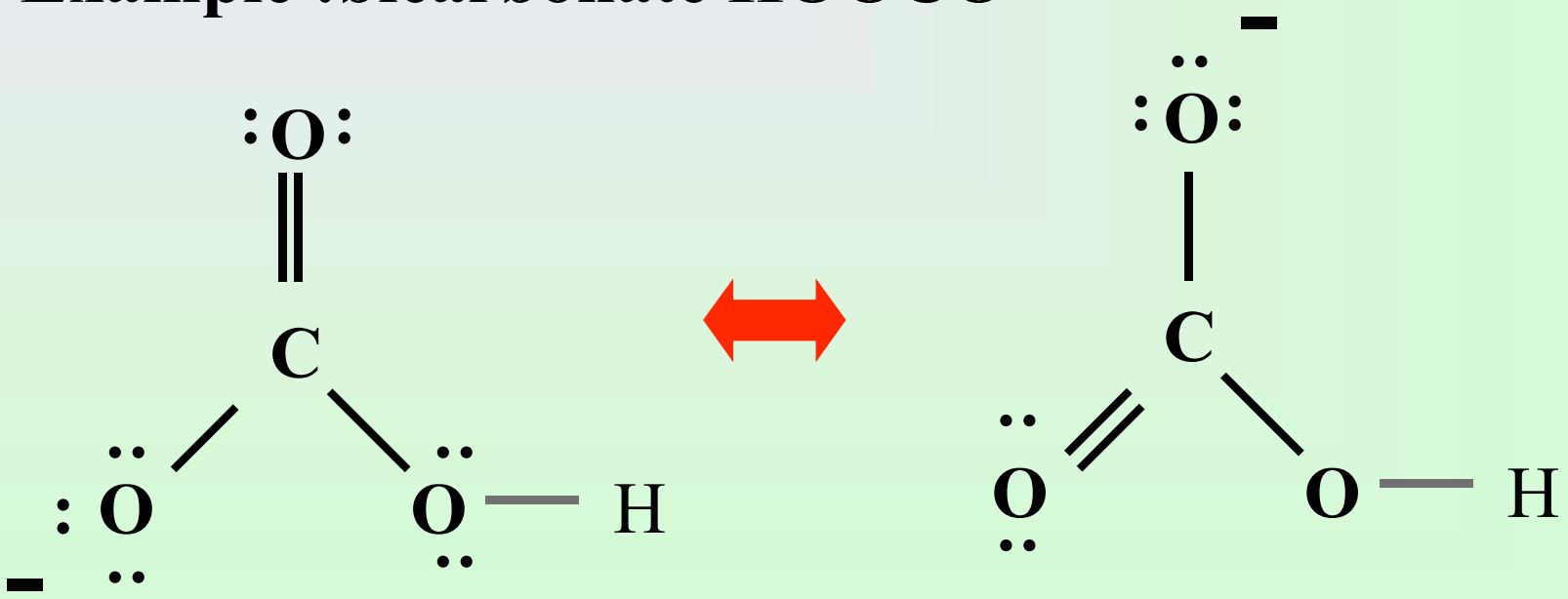


What writing resonance structures accomplishes

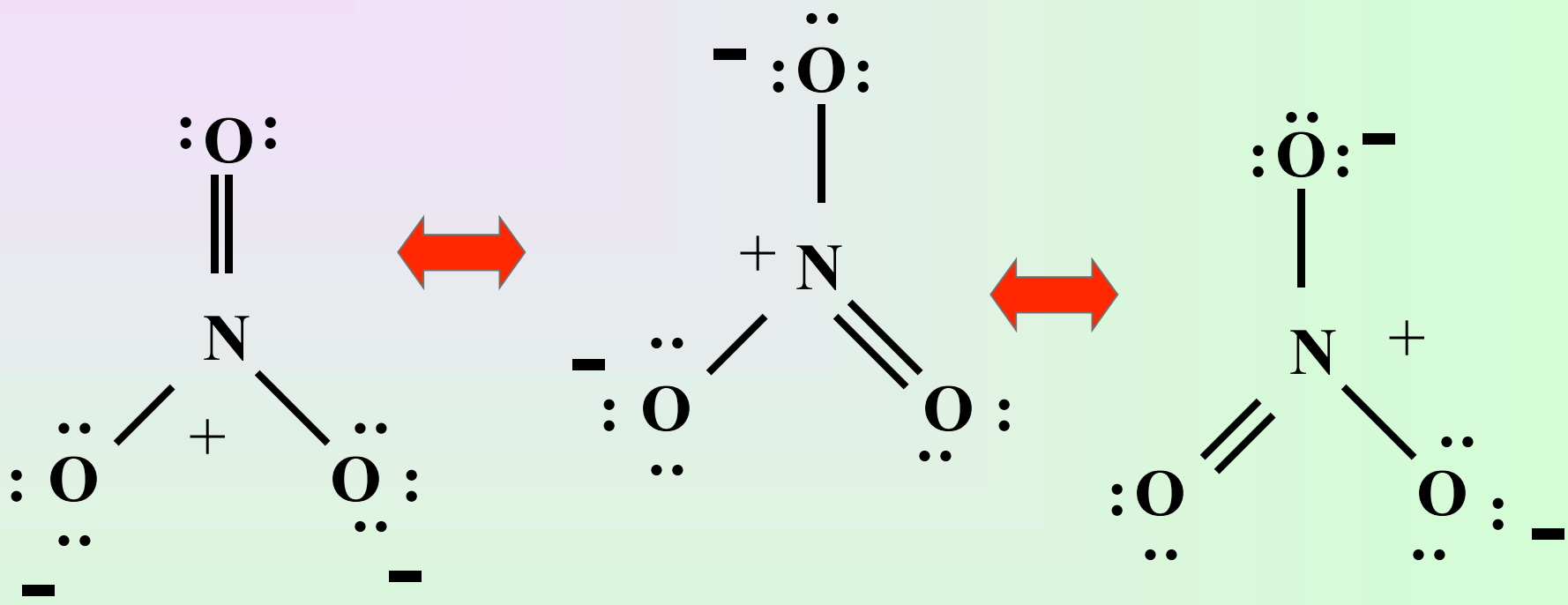
Electrons in molecules are often delocalized between two or more atoms.

electrons in a single Lewis structure are assigned to specific atoms "localization".

a single Lewis Structure is insufficient to show electron delocalization.

a composite of resonance forms more accurately depicts electron distribution

Example



Nitrate ion

Exceptions to the octet rule

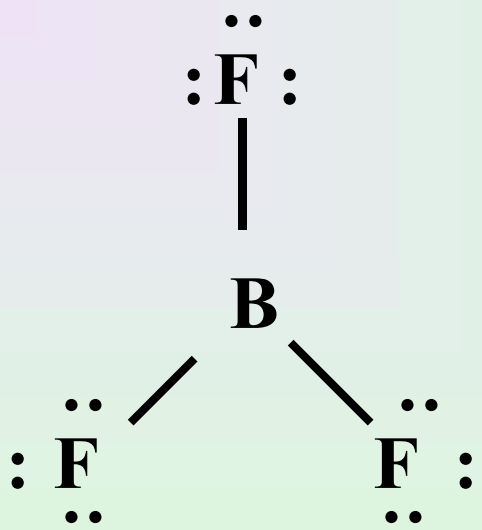
Counting only valence electrons

elements in the second period *can never* have more than 8 electrons

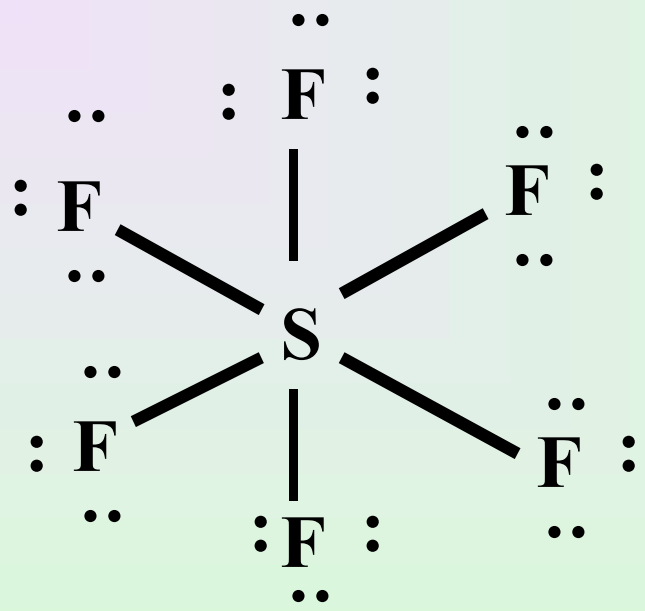
but can have fewer than 8

elements in the third period *can* have more than 8 electrons

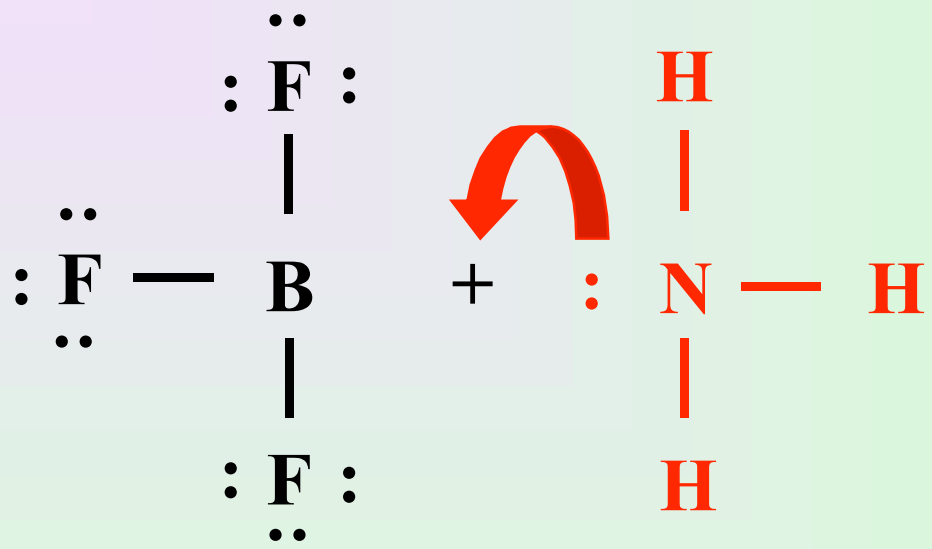
Less than 8 electrons



more than 8 electrons

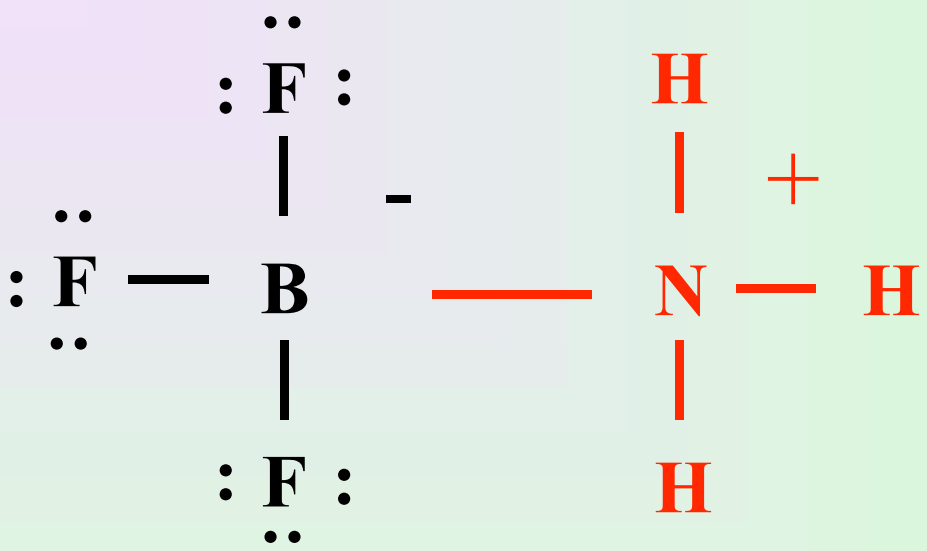


Coordinate Covalent Bond



A covalent bond in which one of the atoms donates both electrons

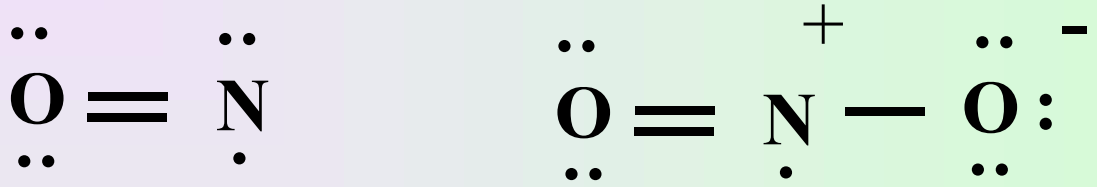
Coordinate Covalent Bond



A covalent bond in which one of the atoms donates both electrons

The distinction is useful for keeping track of electrons and assigning formal charge

Odd Electron Molecules



Some molecules contain an *odd* number of electrons (NO) and (NO_2) notable examples

The octet is not complete