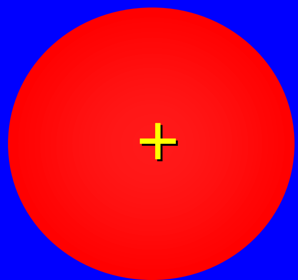
Chapter 1
Chemical Bonding

1.1

Atoms, Electrons, and Orbitals

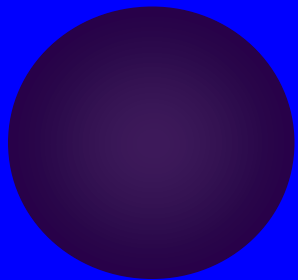
Atoms are composed of



Protons

positively charged

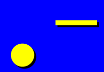
mass = 1.6726 X 10^{-27} kg



Neutrons

neutral

mass = 1.6750 X 10^{-27} kg



Electrons

negatively charged

mass = 9.1096 X 10^{-31} kg

Atomic Number and Mass Number

$${}^{A}_{Z}X$$

Atomic number (Z) = number of protons in nucleus

(this must also equal the number of electrons in neutral atom)

Mass number (A) = sum of number of protons + neutrons in nucleus

Schrödinger Equation

Schrödinger combined the idea that an electron has wave properties with classical equations of wave motion to give a wave equation for the energy of an electron in an atom.

Wave equation (Schrödinger equation) gives a series of solutions called wave functions (y).

Wave Functions

Only certain values of y are allowed.

Each y corresponds to a certain energy.

The probability of finding an electron at a particular point with respect to the nucleus is given by y^2.

Each energy state corresponds to an orbital.

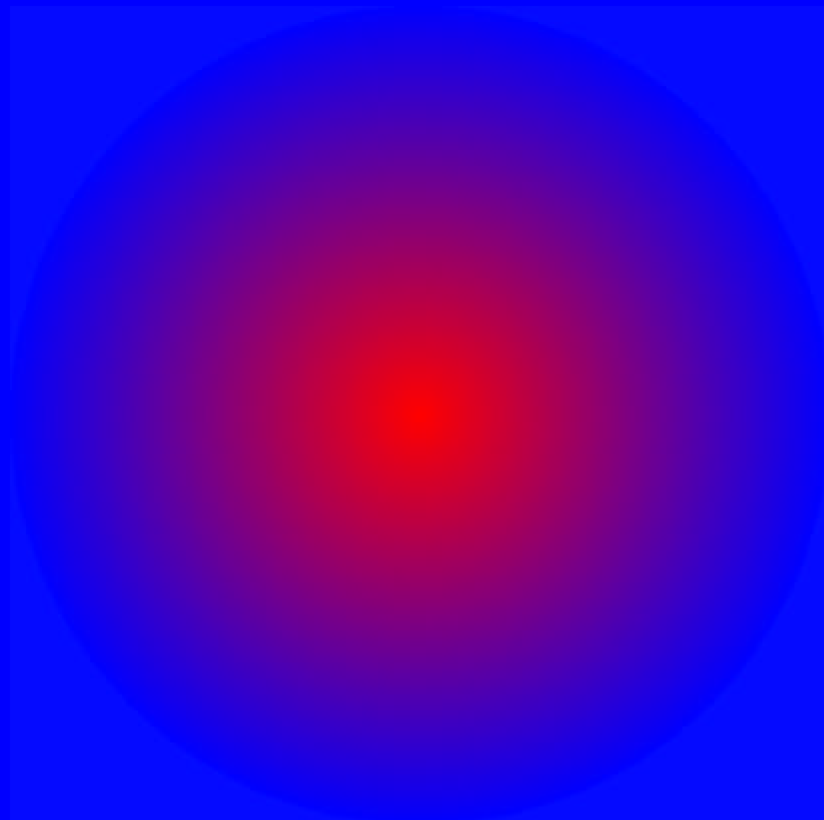
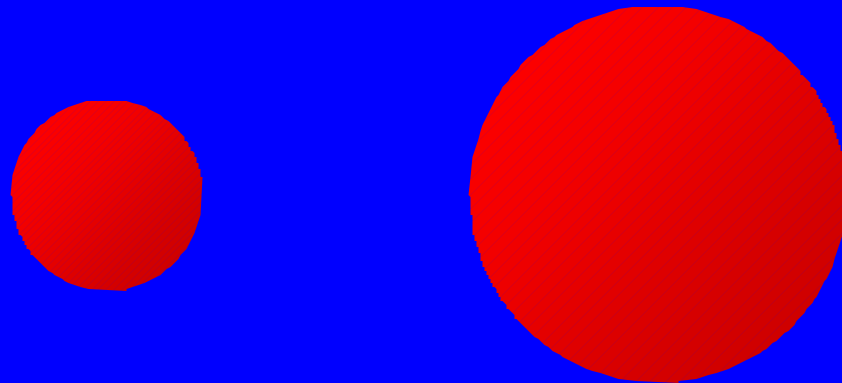


Figure 1.1 Probability distribution (y^2) for an electron in a 1*s* orbital.

A boundary surface encloses the region where the probability of finding an electron is high—on the order of 90-95%



1s 2s

Figure 1.3 Boundary surfaces of a 1*s* orbital and a 2*s* orbital.

Quantum Numbers

Each orbital is characterized by a unique set of quantum numbers.

The principal quantum number *n* is a whole number (integer) that specifies the shell and is related to the energy of the orbital.

The angular momentum quantum number is usually designated by a letter (*s*, *p*, *d*, *f*, etc) and describes the shape of the orbital.

s Orbitals

s Orbitals are spherically symmetric.

The energy of an *s* orbital increases with the number of nodal surfaces it has.

A nodal surface is a region where the probability of finding an electron is zero.

A 1*s* orbital has no nodes; a 2*s* orbital has one; a 3*s* orbital has two, etc.

The Pauli Exclusion Principle

No two electrons in the same atom can have the same set of four quantum numbers.

Two electrons can occupy the same orbital only when they have opposite spins.

There is a maximum of two electrons per orbital.

First Period

Principal quantum number (*n*) = 1

	Hydrogen	Helium
	Z = 1	Z = 2
	$1s^{1}$	$1s^{2}$

	$1s$	$2s$	$2p$		
H	↑				
He	↑↓				

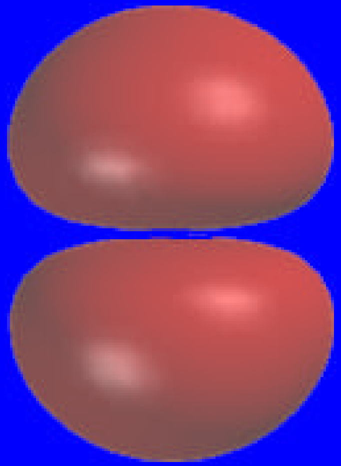
p *Orbitals*

p Orbitals are shaped like dumbells.

Are not possible for *n* = 1.

Are possible for *n* = 2 and higher.

There are three p orbitals for each value of *n* (when *n* is greater than 1).



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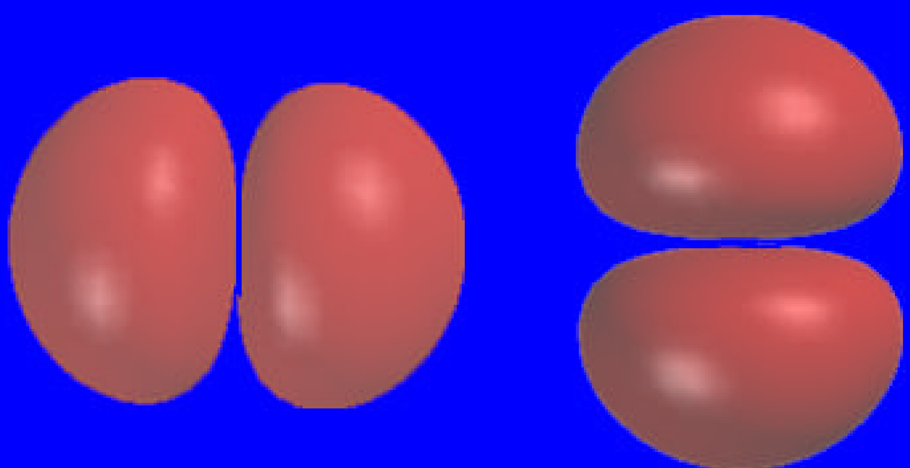

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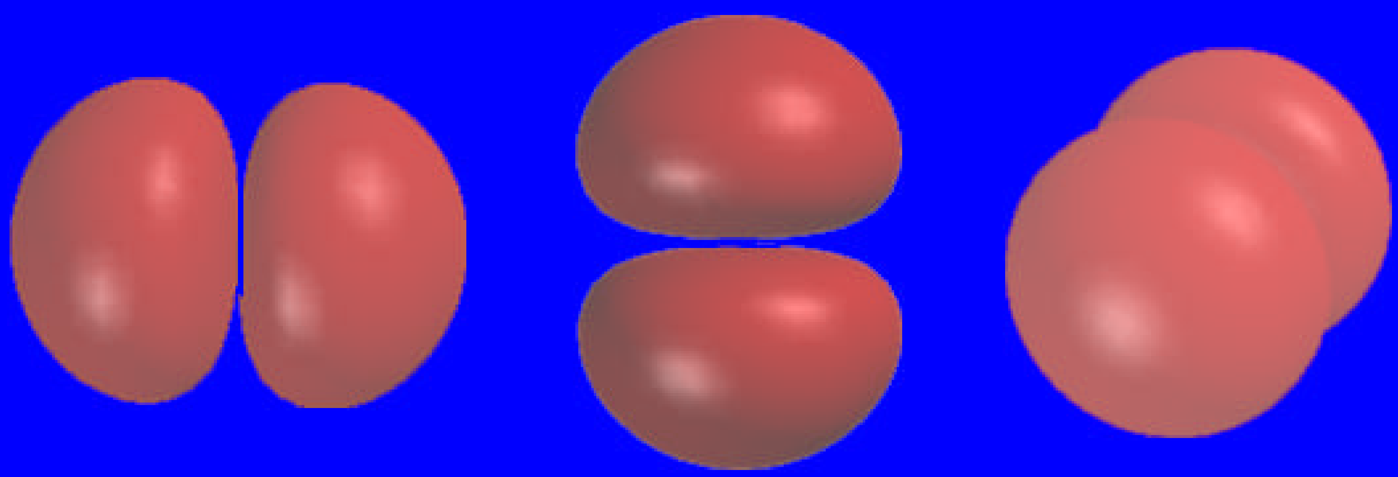


Second Period

Principal quantum number (*n*) = 2

	Z	1*s*	2*s*	2*p*		
Li	3	↑↓	↑			
Be	4	↑↓	↑↓			
B	5	↑↓	↑↓	↑		
C	6	↑↓	↑↓	↑	↑	

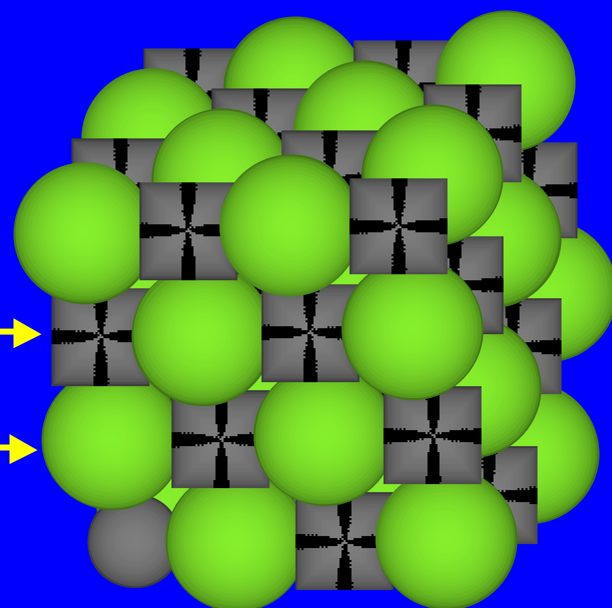
Second Period

	Z	1*s*	2*s*	2*p*
N	7	↑↓	↑↓	↑ | ↑ | ↑
O	8	↑↓	↑↓	↑↓ | ↑ | ↑
F	9	↑↓	↑↓	↑↓ | ↑↓ | ↑
Ne	10	↑↓	↑↓	↑↓ | ↑↓ | ↑↓

1.2
Ionic Bonds

Ionic Bonding

An ionic bond is the force of electrostatic attraction between oppositely charged ions



Na^+ (cation)

Cl^- (anion)

Ionic Bonding

Ionic bonds are common in inorganic chemistry but rare in organic chemistry.

Carbon shows less of a tendency to form cations than metals do, and less of a tendency to form anions than nonmetals.

1.3

Covalent Bonds

The Lewis Model of Chemical Bonding

In 1916 G. N. Lewis proposed that atoms combine in order to achieve a more stable electron configuration.

Maximum stability results when an atom is isoelectronic with a noble gas.

An electron pair that is shared between two atoms constitutes a covalent bond.

Covalent Bonding in H_2

Two hydrogen atoms, each with 1 electron,

$$H\cdot \qquad \cdot H$$

can share those electrons in a covalent bond.

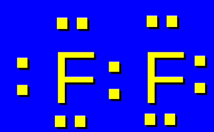
$$H:H$$

Sharing the electron pair gives each hydrogen an electron configuration analogous to helium.

Covalent Bonding in F_2

Two fluorine atoms, each with 7 valence electrons,

can share those electrons in a covalent bond.



Sharing the electron pair gives each fluorine an electron configuration analogous to neon.

The Octet Rule

In forming compounds, atoms gain, lose, or share electrons to give a stable electron configuration characterized by 8 valence electrons.

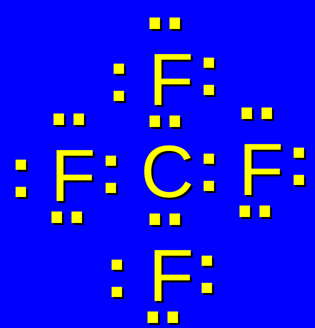
$$:\underset{\cdot\cdot}{\overset{\cdot\cdot}{F}}:\underset{\cdot\cdot}{\overset{\cdot\cdot}{F}}:$$

The octet rule is the most useful in cases involving covalent bonds to C, N, O, and F.

Example

Combine carbon (4 valence electrons) and four fluorines (7 valence electrons each)

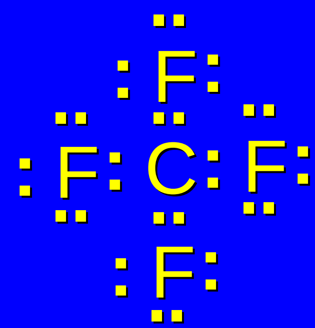
to write a Lewis structure for CF_4.



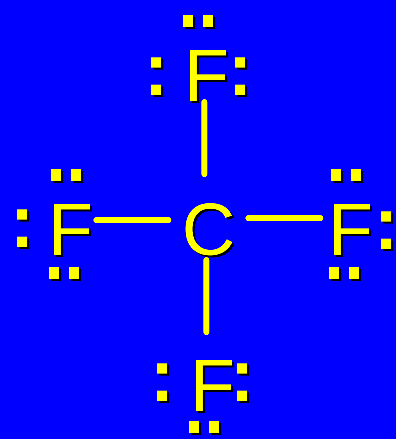
The octet rule is satisfied for carbon and each fluorine.

Example

It is common practice to represent a covalent bond by a line. We can rewrite



as



1.4
Double Bonds and Triple Bonds

Inorganic Examples

$$:\ddot{O}::C::\ddot{O}: \qquad :\ddot{O}=C=\ddot{O}:$$

Carbon dioxide

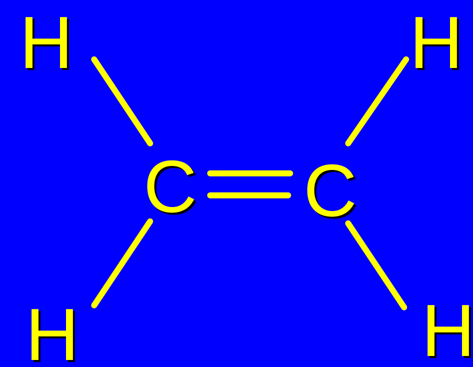
$$H:C:::N: \qquad H-C\equiv N:$$

Hydrogen cyanide

Organic Examples

H   H
¨   ¨
H : C : : C : H

Ethylene



H : C : : : C : H

Acetylene

$H-C\equiv C-H$

1.5
Polar Covalent Bonds and Electronegativity

Electronegativity

Electronegativity is a measure of the ability of an element to attract electrons toward itself when bonded to another element.

An electronegative element attracts electrons.

An electropositive element releases electrons.

Pauling Electronegativity Scale

Li	**Be**	**B**	**C**	**N**	**O**	**F**
1.0	**1.5**	**2.0**	**2.5**	**3.0**	**3.5**	**4.0**
Na	**Mg**	**Al**	**Si**	**P**	**S**	**Cl**
0.9	**1.2**	**1.5**	**1.8**	**2.1**	**2.5**	**3.0**

Electronegativity increases from left to right in the periodic table.

Electronegativity decreases going down a group.

Generalization

The greater the difference in electronegativity between two bonded atoms; the more polar the bond.

H—H　　　:F—F:　　　:N≡N:

nonpolar bonds connect atoms of the same electronegativity

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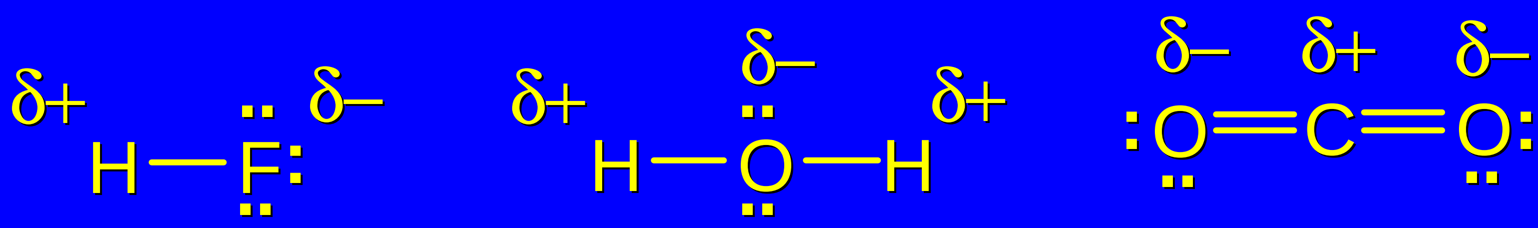


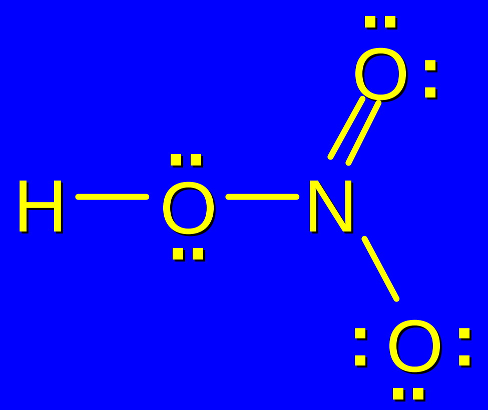
polar bonds connect atoms of different electronegativity

1.6
Formal Charge

Formal charge is the charge calculated for an atom in a Lewis structure on the basis of an equal sharing of bonded electron pairs.

Nitric acid

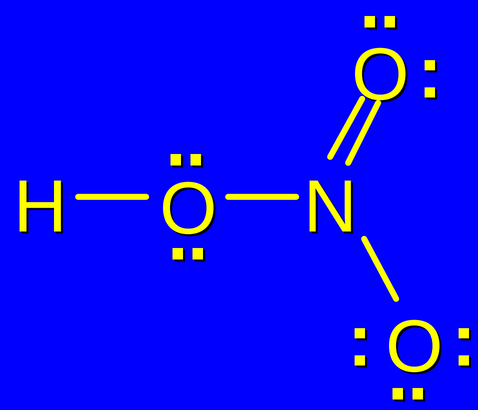
Formal charge of H



We will calculate the formal charge for each atom in this Lewis structure.

Nitric acid

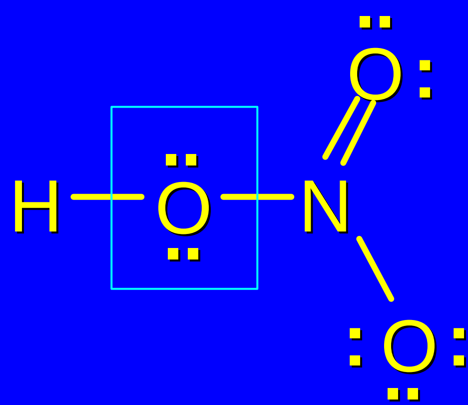
Formal charge of H



- Hydrogen shares 2 electrons with oxygen.
- Assign 1 electron to H and 1 to O.
- A neutral hydrogen atom has 1 electron.
- Therefore, the formal charge of H in nitric acid is 0.

Nitric acid

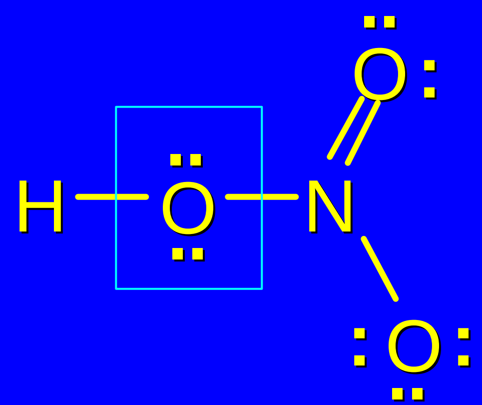
Formal charge of O



- Oxygen has 4 electrons in covalent bonds.
- Assign 2 of these 4 electrons to O.
- Oxygen has 2 unshared pairs. Assign all 4 of these electrons to O.
- Therefore, the total number of electrons assigned to O is 2 + 4 = 6.

Nitric acid

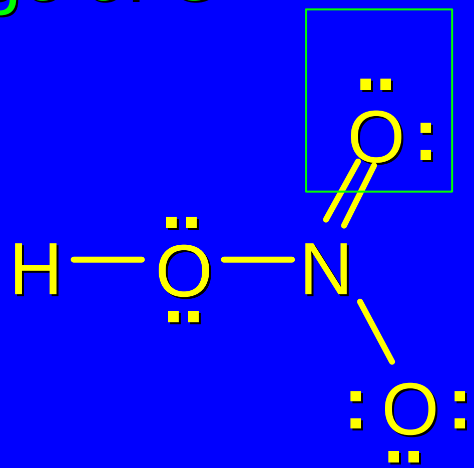
Formal charge of O



- Electron count of O is 6.
- A neutral oxygen has 6 electrons.
- Therefore, the formal charge of O is 0.

Nitric acid

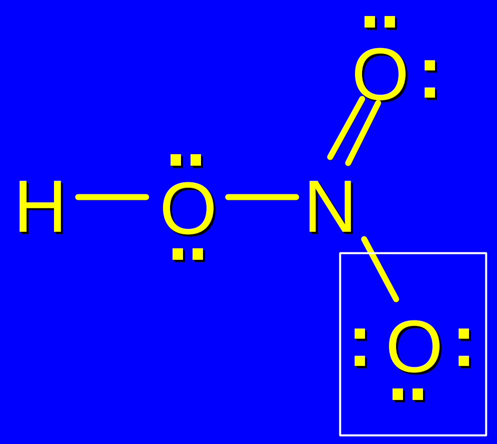
Formal charge of O



- Electron count of O is 6 (4 electrons from unshared pairs + half of 4 bonded electrons).
- A neutral oxygen has 6 electrons.
- Therefore, the formal charge of O is 0.

Nitric acid

Formal charge of O



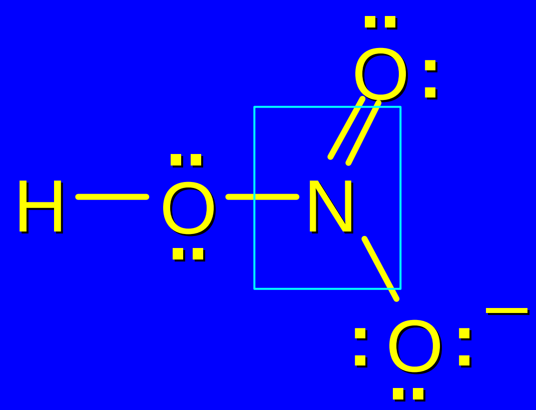
•Electron count of O is 7 (6 electrons from unshared pairs + half of 2 bonded electrons).

•A neutral oxygen has 6 electrons.

•Therefore, the formal charge of O is -1.

Nitric acid

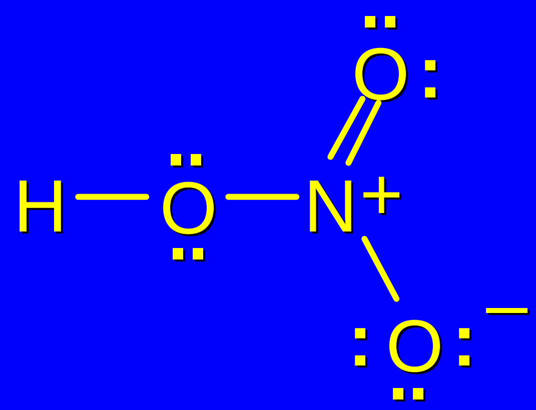
Formal charge of N



- Electron count of N is 4 (half of 8 electrons in covalent bonds).
- A neutral nitrogen has 5 electrons.
- Therefore, the formal charge of N is +1.

Nitric acid

Formal charges



•A Lewis structure is not complete unless formal charges (if any) are shown.

Formal Charge

An arithmetic formula for calculating formal charge.

Formal charge =

group number in periodic table – number of bonds – number of unshared electrons

Formal Charge

"Electron counts" and formal charges in NH_4^+ and BF_4^-