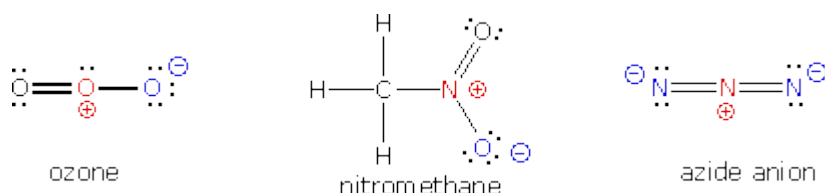


Charge Distribution and Functional Groups

If the electron pairs in covalent bonds were donated and shared absolutely evenly there would be no fixed local charges within a molecule. Although this is true for diatomic elements such as H₂, N₂ and O₂, most covalent compounds show some degree of local charge separation, resulting in bond and / or molecular dipoles. A dipole exists when the centers of positive and negative charge distribution do not coincide.

Formal Charges

A large local charge separation usually results when a shared electron pair is donated unilaterally. The three Kekulé formulas shown here illustrate this condition.



In the formula for ozone the central oxygen atom has three bonds and a full positive charge while the right hand oxygen has a single bond and is negatively charged. The overall charge of the ozone molecule is therefore zero. Similarly, nitromethane has a positive-charged nitrogen and a negative-charged oxygen, the total molecular charge again being zero. Finally, azide anion has two negative-charged nitrogens and one positive-charged nitrogen, the total charge being minus one. In general, for covalently bonded atoms having valence shell electron octets, if the number of covalent bonds to an atom is greater than its normal valence it will carry a positive charge. If the number of covalent bonds to an atom is less than its normal valence it will carry a negative charge. The formal charge on an atom may also be calculated by the following formula:

$$\text{Formal Charge} = \text{Valence Electrons in Neutral Atom} - \left(\text{Unshared Valence Electrons} + \text{Half of the Shared Electrons} \right)$$

Polar Covalent Bonds

H	Electronegativity for Some Elements	Values
2.20		

Because of their differing nuclear charges, and as a result of shielding by inner electron shells, the different atoms of the periodic table have different affinities for nearby electrons. The ability of an element to attract or hold onto electrons is called **electronegativity**. A rough quantitative scale of

Li 0.98	Be 1.57	B 2.04	C 2.55	N 3.04	O 3.44	F 3.98
Na 0.90	Mg 1.31	Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16
K 0.82	Ca 1.00	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96

electronegativity values was established by [Linus Pauling](#), and some of these are given in the table to the right. A larger number on this scale signifies a greater affinity for electrons. Fluorine has the greatest electronegativity of all the elements, and the heavier alkali metals such as potassium, rubidium and cesium have the lowest electronegativities. It should be noted that carbon is about in the middle of the electronegativity range, and is slightly more electronegative than hydrogen. When two different atoms are bonded covalently, the shared electrons are attracted to the more electronegative atom of the bond, resulting in a shift of electron density toward the more electronegative atom. Such a covalent bond is **polar**, and will have a **dipole** (one end is positive and the other end negative). The degree of polarity and the magnitude of the bond dipole will be proportional to the difference in electronegativity of the bonded atoms. Thus a O–H bond is more polar than a C–H bond, with the hydrogen atom of the former being more positive than the hydrogen bonded to carbon. Likewise, C–Cl and C–Li bonds are both polar, but the carbon end is positive in the former and negative in the latter. The dipolar nature of these bonds is often indicated by a partial charge notation ($\delta+/-$) or by an arrow pointing to the negative end of the bond.



Although there is a small electronegativity difference between carbon and hydrogen, the C–H bond is regarded as weakly polar at best, and hydrocarbons in general are considered to be non-polar compounds.

The shift of electron density in a covalent bond toward the more electronegative atom or group can be observed in several ways. For bonds to hydrogen, acidity is one criterion. If the bonding electron pair moves away from the hydrogen nucleus the proton will be more easily transferred to a base (it will be more acidic). A comparison of the acidities of methane, water and hydrofluoric acid is instructive. Methane is essentially non-acidic, since the C–H bond is nearly non-polar. As noted above, the O–H bond of water is polar, and it is at least 25 powers of ten more acidic than methane. H–F is over 12 powers of ten more acidic than water as a consequence of the greater electronegativity difference in its atoms. Electronegativity differences may be transmitted through connecting covalent bonds by an **inductive effect**. Replacing one of the hydrogens of water by a more electronegative atom increases the acidity of the remaining O–H bond. Thus hydrogen peroxide, HO–O–H, is ten thousand times more acidic than water, and hypochlorous acid, Cl–O–H is one hundred million times more acidic. This inductive transfer of polarity tapers off as the

number of transmitting bonds increases, and the presence of more than one highly electronegative atom has a cumulative effect. For example, trifluoro ethanol, $\text{CF}_3\text{CH}_2\text{O}-\text{H}$ is about ten thousand times more acidic than ethanol, $\text{CH}_3\text{CH}_2\text{O}-\text{H}$.

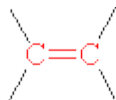

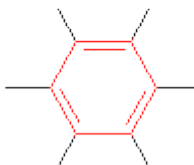
Excellent physical evidence for the **inductive effect** is found in the influence of electronegative atoms on the [nmr chemical shifts](#) of nearby hydrogen atoms.

Functional Groups


Functional groups are atoms or small groups of atoms (two to four) that exhibit a characteristic reactivity when treated with certain reagents. A particular functional group will almost always display its characteristic chemical behavior when it is present in a compound. Because of their importance in understanding organic chemistry, functional groups have characteristic names that often carry over in the naming of individual compounds incorporating specific groups. In the following table the atoms of each functional group are colored red and the characteristic IUPAC nomenclature suffix that denotes some (but not all) functional groups is also colored.


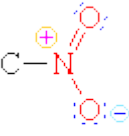
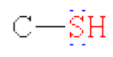
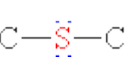
Functional Group Tables

Exclusively Carbon Functional Groups


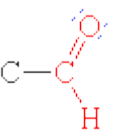
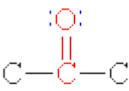
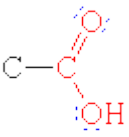
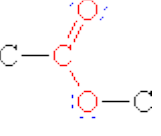
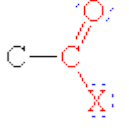
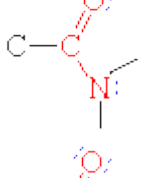
Group Formula	Class Name	Specific Example	IUPAC Name	Common Name
	Alkene	$\text{H}_2\text{C}=\text{CH}_2$	Ethene	Ethylene
	Alkyne	$\text{HC}\equiv\text{CH}$	Ethyne	Acetylene
	Arene	C_6H_6	Benzene	Benzene

Functional Groups with Single Bonds to Heteroatoms

Group Formula	Class	Name	Specific Example	IUPAC Name	Common Name
	Halide		$\text{H}_3\text{C}-\text{I}$	Iodomethane	Methyl iodide

	Alcohol	$\text{CH}_3\text{CH}_2\text{OH}$	Ethan ol	Ethyl alcohol
	Ether	$\text{CH}_3\text{CH}_2\text{OCH}_2\text{CH}_3$	Diethyl ether	Ether
	Amine	$\text{H}_3\text{C-NH}_2$	Aminomethane	Methylamine
	Nitro Compound	$\text{H}_3\text{C-NO}_2$	Nitromethane	
	Thiol	$\text{H}_3\text{C-SH}$	Methan ethiol	Methyl mercaptan
	Sulfide	$\text{H}_3\text{C-S-CH}_3$	Dimethyl sulfide	

Functional Groups with Multiple Bonds to Heteroatoms

Group Formula	Class Name	Specific Example	IUPAC	Name Common	Name
	Nitrile	$\text{H}_3\text{C-CN}$	Ethanenitrile	Acetonitrile	
	Aldehyde	H_3CCHO	Ethan al	Acetaldehyde	
	Ketone	H_3CCOCH_3	Propan one	Acetone	
	Carboxylic Acid	$\text{H}_3\text{CCO}_2\text{H}$	Ethan oic Acid	Acetic acid	
	Ester	$\text{H}_3\text{CCO}_2\text{CH}_2\text{CH}_3$	Ethyl ethan oate	Ethyl acetate	
	Acid Halide	H_3CCOCl	Ethan oyl chloride	Acetyl chloride	
	Amide	$\text{H}_3\text{CCON}(\text{CH}_3)_2$	N,N-Dimethylethanamide	N,N-Dimethylacetamide	

Acid Anhydride $(\text{H}_3\text{CCO})_2\text{O}$ Ethanoic anhydride Acetic anhydride

Source :<http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro2.htm#start>