**Rules for Drawing Resonance Structures**

Resonance

1. Often a single Lewis structure does not accurately represent the true structure of a molecule. Case in point is the carbonate anion (CO32-).
2. First draw the best Lewis structure.
3. The real carbonate ion is not represented by any of the structures 1,2 or 3



1. Experimentally carbonate is known not to have two carbon-oxygen single bonds and one double bond; all bonds are equal in length and the charge is spread equally over all three oxygens
2. The real carbonate ion can be represented by a drawing in which partial double bonds to the oxygens are shown and partial negative charge exists on each oxygen
3. The real structure is a resonance hybrid or mixture of all three Lewis structures
4. Double headed arrows are used to show that the three Lewis structures are resonance contributors to the true structure
	1. The use of equilibrium arrows is incorrect since the three structures do not equilibrate; the true structure is a hybrid (average) of all three Lewis structures



1. One resonance contributor is converted to another by the use of curved arrows which show the movement of electrons
	1. The use of these arrows serves as a bookkeeping device to assure all structures differ only in position of electrons



1. A calculated electrostatic potential map of carbonate clearly shows the electron density is spread equally among the three oxygens
	1. Areas which are red are more negatively charged; areas of blue have relatively less electron density



Rules for Resonance

1. Individual resonance structures exist only on paper
	1. The real molecule is a hybrid (average) of all contributing forms
	2. Resonance forms are indicated by the use of double-headed arrows
2. Only electrons are allowed to move between resonance structures
	1. The position of nuclei must remain the same
		1. The sigma bond framework remains unaltered
	2. Only electrons in multiple bonds and nonbonding electrons can be moved
	3. Permitted electron movements are:
		1. Bond to adjacent bond



* + 1. Bond to adjacent atom



* + 1. Atom to adjacent bond



1. Example: 3 is not a resonance form because an atom has moved



1. All structures must be proper Lewis structures



1. The energy of the actual molecule is lower than the energy of any single contributing form
	1. The lowering of energy is called resonance stabilization or resonance energy (R.E.)
	2. The more resonance forms that can be drawn, the lower the energy – greater the stability of the hybrid
	3. R.E. is defined as the difference in energy between the energy of the hybrid structure and the energy of the most stable resonance form
2. Equivalent resonance forms make equal contributions to the structure of the real molecule
	1. Resonance structures are equivalent when they have the same number of bonds, unshared pairs of electrons, and the same charge, but otherwise are different structures by either location of a double bond or charge
	2. Structures with equivalent resonance forms are degenerate in energy and tend to be greatly stabilized
	3. Example: The two resonance forms of benzene contribute equally and greatly stabilize it



 Energy diagram representation:



1. Unequal resonance structures contribute based on their relative stabilities
	1. More stable resonance forms contribute more to the structure of the real molecule



δ+

δ-

hybrid representation



* 1. Note in the above examples, the R.E. for benzene is much greater than that obtained for the amide

Rules to Assign Relative Importance of Resonance Forms

1. A resonance form with more covalent bonds is more important than one with less
	1. Example: 6 is more stable and more important because it has more total covalent bonds



1. Resonance forms in which all atoms have a complete valence shell of electrons are more important
	1. Example: 10 is more important because all atoms (except hydrogen) have complete octets



1. Resonance forms with separation of charge are less important
	1. Resonance forms with the fewest number of formal charges are preferred and of lower energy
	2. Separation of charge cost energy and results in a less stable resonance contributor
	3. Example: 12 is less important because it has charge separation



1. Forms with negative charge on highly electronegative atoms are more important
	1. Those with positive charge on less electronegative atoms are also more important

Example – NO3-

1. Drawing the best Lewis structure results in the following:



1. The nitrate ion is known to have all three nitrogen-oxygen bond lengths the same and the negative charge spread over all three atoms equally
2. Resonance theory can be used to produce three equivalent resonance forms
	1. Curved arrows show the movement of electrons between forms
	2. When these forms are hybridized (averaged) the true structure of the nitrate ion is obtained



