Non-Equivalent Resonance Structures and Formal Charges

The assignment of formal charges to each atom in a Lewis dot structure can help to determine the relative stability of the structure. Note that formal charges are not the actual charges on the elements, but rather an "exaggerated charge" that assumes perfect sharing of electrons.

For a particular atom in a covalently bonded molecule or ion:

F.C. = # of valence electrons in free atom – [# of bonds to atom + # of lone electrons]

How do you use formal charges to find the most stable non-equivalent resonance structure?
The most stable structure is the one with:

a) the lowest sum when the absolute values of the formal charges are added

b) the largest negative formal charge on the most electronegative element (when 2 or more structures have the same lowest sum)

A classic illustrative example

For SCN^-, three non-equivalent resonance structures are possible:

I	II	III
$[:\ddot{\underset{..}{S}}-C\equiv N:]^-$	$[:\ddot{S}=C=\ddot{N}:]^-$	$[:S\equiv C-\ddot{\underset{..}{N}}:]^-$

For structure 1: F.C. S = 6 – [1 + 6] = –1
F.C. C = 4 – [4 + 0] = 0 Absolute sum = 1 + 0 + 0 = 1
F.C. N = 5 – [3 + 2] = 0

For structure 2: F.C. S = 6 – [2 + 4] = 0
F.C. C = 4 – [4 + 0] = 0 Absolute sum = 0 + 0 + 1 = 1
F.C. N = 5 – [2 + 4] = –1

For structure 3: F.C. S = 6 – [3 + 2] = 1
F.C. C = 4 – [4 + 0] = 0 Absolute sum = 1 + 0 + 2 = 3
F.C. N = 5 – [1 + 6] = –2

Based on the absolute sum of the formal charges, structures 1 and 2 seem to be equally favorable. Nevertheless, N is more electronegative than S, so by Rule b above, structure 2 is the most favorable of the three.

* (1) CLOSEST TO ZERO WINS (2) IF TWO WIN, THEN ONE w/ "–" FC ON MOST E-NEG ELEMENT WINS!!

Valence Rules

Based on the formal charge rules, we can assign so-called valence rules to the nonmetal elements. The valence rules can help to determine arrangement of atoms in a molecule.

Atom(s)	Preferred number of bonds
C	4
N	3
S, O	2
Halogens	1