

Rules of thumb for predicting the relative stabilities of molecules (or resonance forms)

These rules are in approximate order of importance.

1. Octet rule. Having 8 valence electrons around an atom (2 in the case of H) is a particularly stable arrangement. Atoms in the second period (C, N, O, F) never exceed an octet. Atoms in the third period and above may exceed octet (P, S, Cl, etc., up to 12 electrons).

Molecules without octets are normally very reactive. (e.g. carbocations, carbenes, BF_3)

2. Minimize formal charge. Molecules (or resonance forms) with more or larger formal charges on atoms are less stable (i.e. more reactive) than corresponding molecules lacking those charges (or with the charges delocalized.)

Corollary: Most Lewis structures of neutral molecules (molecules with no charge) have no formal charges on any of the atoms. (There are a few exceptions to this.)

For neutral atoms (no formal charge) the number of bonds usually equals the number of electrons the atom needs to get to a noble gas arrangement: C=4, N=3, O=2, F=1 (Except for those that don't follow octet rule.)

Electron withdrawing groups stabilize adjacent negative charges, destabilize adjacent positive. ("Inductive effect")

3. Negative on Electronegative. Molecules (or resonance forms) with the negative charge on a more electronegative atom (and conversely positive charges on more electropositive atoms) are more stable than the alternatives.

Exception: For atoms in different rows, having a negative charge on the larger atom is often preferable.

See problems 8 and 9 in worksheet 1.

4. Resonance stabilizes. Delocalization of electrons is stabilizing.

Compare acidity of ethanol and phenol and acetate.

5. Inductive effects. Electron withdrawing groups stabilize adjacent negative charges, destabilize adjacent positive. Opposite for electron donating groups.

6. 3-dimensional arrangement of atoms influences stability

Strain destabilizes a molecule (3 or 4-membered rings e.g.)