SECTION 5

STRUCTURAL FORMULAE

Structural formula: A chemical formula which shows the groupings of atoms in a compound.

Lewis structures (defined in *section 4*) of discrete molecules and ions are an essential part of the chemical language. They are used to show details of structure and of chemical reactions. The ability to write Lewis structures for basic molecules and ions is an essential skill for chemists. The following rules require knowledge only of the number of valence electrons of an atom of each element, and the arrangement of the nuclei, i.e. which atoms are joined or bonded together.

Rules for Drawing Lewis Structures

(a) Determine the total number of valence electrons in the molecule or ion by adding together the numbers of valence electrons of each atom, and if an anion, by adding the overall charge of the ion, and if a cation, by subtracting the overall charge of the ion.

(b) Place the atoms in their relative positions.

(c) Draw a line representing a single bond containing two electrons between joined atoms.

(d) Distribute the remaining electrons evenly in pairs on the outer atoms so these have up to eight electrons (except for hydrogen which has two). Any still not used after this should be placed on the central atom.

Formal Charge: The electric charge of an atom in a molecule or ion assuming perfect covalent bonding. [e.g. in NH_4^+, N "owns" four electrons and has the formal charge +1 as an N atom has five valence electrons.]

Examples:

Rule	CO_3^{2-}	NO_2	SO_2
a	C O 4 + 3 x 6 + 2 = 24	N O 5 + 2 x 6 = 17	S O 6 + 2 x 6 = 18

molecule or ion is called a **resonance structure**, and the true structure of the molecule or ion is a composite of these called the **resonance hybrid**. (See benzene, *page 6-5*)

Of course, many molecules or ions do not have a "central atom". Organic molecules with more than one C are obvious examples. Provided the structure is known, (i.e. which atoms are bonded to which), extending the rules with common sense will work. [e.g. C_2H_2, H-C-C-H, put pairs on C atoms evenly, and move both pairs to between C atoms to make a triple bond.

H—C≡C—H . Th a l i n 9 g i v e e

atoms. BF_3