

Structure – Property Relationships

Why is a particular drug effective, why is a particular chemical toxic, why does a particular pesticide not break down in the environment, why does a bullet-proof vest work the way it does? The answer to all of these is that the structure of the molecules comprising these materials makes them behave in the way they do.

“**Structure Determines Properties**” is a powerful concept in chemistry and all fields in which chemistry is important including, but not limited to, environmental science, biology, biochemistry, polymer science, medicine, and nutrition.

How does one describe the structure of a molecule?

- Molecular formula, e.g., $C_{12}H_{17}ClNO_3$
- Size, 3-Dimensional Shape (steric effects)
- Functional Groups (electrostatic effects - Polarity, H-Bonding)
- Chirality
- Energy of Formation.
- to be precise, the exact structure would require defining the exact positions of all atoms in the molecule.

What is meant by properties?

- chemical (e.g., reaction rates, position of equilibria)
- physical (e.g., melting points, boiling points, solubility, spectra)
- biological (e.g., odor, color, taste, drug action, toxicity)

How structure affects properties, some examples.

Compare dimethyl ether, CH_3-O-CH_3 (bp -24°) and its isomer, ethanol, CH_3CH_2-O-H (bp 78°). In this case the structures determine the boiling points. The molecules of alcohol, having the ability to H-bond, attract one another with stronger forces (H-bonds) than do the molecules of ether which only have normal dipole-dipole forces holding them together.

Compare the enantiomers of thalidomide. One is an effective antidepressant while the other is mutagenic. Why might this be? The biologically active sites in living systems are chiral themselves. Thus enantiomers can fit differently into those sites and have different biological effects.