

“Structure Determines Properties”

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)