

Molecular Models as Representations of Molecular Structure

Organic molecules are three-dimensional (3D) objects, not the 2D line-angle drawings that we write on a piece of paper. The ability to interpret line-angle drawings as 3D objects is a learned skill. Just like any other skill, you will need to practice if you expect to become proficient at the task. To facilitate the development of this skill, students must take an active role in the learning process, by using physical models (i.e., plastic molecular model kits) and / or software that aid 3D visualization. These visualization aids will help you understand the relationship between a molecule's three dimensional structure and its two dimensional projection.

- Positively charged **nuclei** define atomic positions as {x, y, z} Cartesian coordinates
- Negatively charged **electron cloud** (diffuse entity) defines a molecule's size & shape



acetylene



wireframe



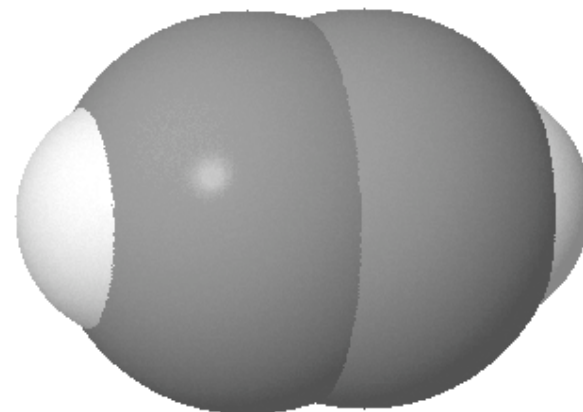
ball & stick

The “ball and stick” model represents each atom as a small sphere and each covalent bond as a cylinder. The “sticks” or “wireframe” rendering is a nice way to view the molecular skeleton without a lot of clutter.



Spacefilling Models

The size and shape of a molecule is determined by the space occupied by its atoms. A hard sphere is the model frequently used to represent the shape of atoms. One useful measure of the size of atoms is the so-called van der Waals radius.



acetylene

This diagram illustrates the relationship between bond distance (1.08 Å) and van der Waals radii (1.20 Å and 1.70 Å) for a hydrogen atom and a carbon atom in acetylene. Only a small portion of the hydrogen atom's sphere will be visible since the size of carbon is much larger.

