6.1: Introduction to Conformation

When we smell something, the information travels to us via molecules, and almost always these are organic molecules. These molecules can be detected by a variety of organs, including noses in dogs and antennae in crickets, but no matter what organ is sensing the smell, one of the crucial factors in determining how an organism reacts to a compound is the shape of the molecule. The sense of smell depends on thousands of different receptors in the organ, working conceptually on a lock-and-key basis: a molecule with a given shape can fit into a given receptor, and when it does, a signal is sent telling the nervous system that the organism has encountered that particular type of molecule, and the organism reacts appropriately.

What gives a molecule its shape? Given a structural formula, could you determine the shape of the corresponding molecule in three dimensions? Could you predict its biological activity, including not only its smell, but also a host of other behaviors linked to the shape of molecular messengers, such as anti-cancer activity or narcotic properties? These questions are at the cutting edge of biological chemistry. Although they are best answered through computer modeling, we can develop some of the qualitative ideas used in these models.

Computer modeling employs "basis sets", small sets of information that the computer could apply to any molecule in order to predict its properties. In order to understand computational conformational analysis, in this chapter we will develop a very simple basis set as an example.