

Molecular Lattices

Here we would like to apply what we discovered about two and three dimensional lattices to different molecular structures. In particular, atoms which can form long linear strings or large two and/or three dimensional patterns should be very special and, in turn, give rise to some very interesting physical substances.

1. Which atoms can, in principle, combine in long, linear strings? What properties would you expect from such a substance (assuming it is liquid or solid)? What symmetries would you expect to find?

2. Here are some specific examples of the type of behavior indicated in Problem 1 although we will allow two different constituent atoms in the molecules. The family of molecules in this problem are called *alkanes* and they consist of strings of carbon atoms bonded with hydrogen atoms where the bonds between carbon atoms are *single*. In answering these questions, there are two possible approaches: examining symmetry based on the chemical formula and examining symmetry based on experimental evidence for the structure of the given molecules. Of course, those without chemistry background should consider the former only.
- a. The simplest alkane is methane which we have already seen. Recall its chemical structure and symmetries.
 - b. The next simplest alkane is ethane with chemical formula C_2H_6 . Draw a picture of the ethane molecule and find its symmetries.
 - c. The next in the series of alkanes is propane with chemical formula C_3H_8 . Draw a picture of the propane molecule and find its symmetries.
 - d. In general, can one build longer and longer chains by inserting more carbon and hydrogen atoms in the middle? What effect does this have on symmetry?

- 3.** Another common form of hydrocarbons is similar to that seen in problem **2** except that now the carbon atoms form a *ring*, with single bonds between carbon atoms, and then each carbon atom is in addition bonded to two hydrogen atoms.
- Describe the structure and symmetries of cyclopropane, C_3H_6 .
 - Describe the structure and symmetries of cyclobutane, C_4H_8 .
 - As more and more carbon atoms are entered in the ring, what happens to the bonding angle of the carbon atoms? For maximal stability of the ring, how many carbon atoms would you expect?

4. We saw that there are three plane lattice systems made of regular polygons. Can any of these be realized chemically, with a single atom at each vertex? For simplicity, let us suppose that only *one* type of atom (e.g. only oxygen atoms or only nitrogen atoms) is allowed at each vertex and suppose also that we only consider atoms that are bonded ionically or covalently.
- What properties of the three different lattices impose the most severe restrictions?
 - Which atoms could *possibly* form such a lattice in a stable fashion?
 - What properties would you expect from such a substance?

There are additional constraints on the atoms forming two dimensional lattices: in particular bonding angles obey very specific laws and most molecules have three dimensional shapes rather than extending outward in a planar structure.

5. Which of the five Platonic solids would you expect to be realized with a single atom (of fixed kind) located at each vertex? What if you allow slightly more complex structures so that instead of an atom at each vertex you allow a simple molecule?
- Make a table of the important structures of each Platonic solid (numbers of vertices, edges, and faces) and the constraints this imposes on possible bonds.
 - Which atoms could *possibly* form a Platonic solid?
 - Do you think that any of the single atoms which could in principle form a cube would do so in a stable fashion?

6. The compound sulfur hexafluoride has chemical formula SF_6 .
- a. What shape do you expect this molecule to take?
 - *b*. What type of bonds hold this molecule together?