UNIT 1: QUANTUM CHEMISTRY

TOPIC 7: Configuration Diagram Glyphs for Atoms

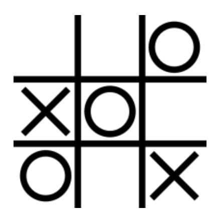
A. We can use fairly simple diagrams to represent atomic orbital occupations that convey their three-dimensional nature.

We will soon move on to discussing the formation of molecules. It will be useful to represent atoms in a manner that indicates orbital occupations and displays their relative orientations. This depiction is limited to s and p valence orbitals, but the main group elements are central to much of chemistry.

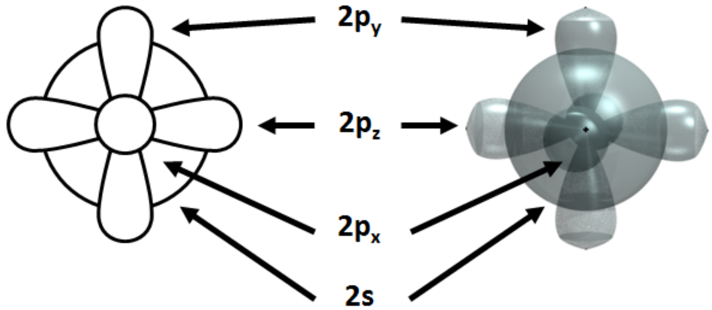
The diagrams that are about to be introduced fall into the large category known as **glyphs**. Each of the various alphabets used in the languages of the world is a family of glyphs. Some are fairly simple, like the English alphabet (26 letters, with capital and lower-case forms, plus punctuation marks). Some are more complex, like the Hanzi used in Chinese language, the Kanji used in Japanese language, and so on. One of the earliest written languages was created in Egypt around 3300 BCE, where the word **hieroglyphs** describes their pictographs.

原子
分子
电子
轨道

We string the glyphs of language together for written communication. Here we will assemble **chemical glyphs** to describe atoms first and then molecules in Unit 2. Just as punctuation and diacritical marks modify characters or sentences, we will start with a few basic forms and "mark them up" to indicate orbital occupations and chemical bonds. A tic tac toe game is a good analogy for this: you start with the basic grid and add X's and O's to it.

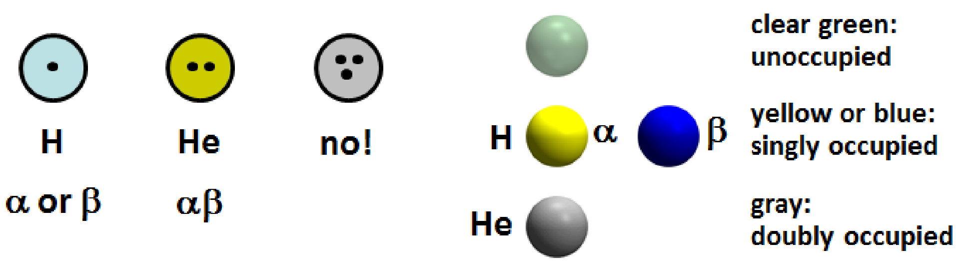


We've noted that an s orbital is spherical and centered on the nucleus, while the three p orbitals are aligned with the cartesian x, y, z axes that are mutually orthogonal; they each possess a node at the nucleus. Two forms of representation of these relationships are shown in the next figure. While both forms are intended to convey the three-dimensional relationships between the p orbitals, the form on the right is a better 3D projection. In the form on the left the out-of-plane 2p orbital is represented by the small inner circle, since we are only seeing the end of the orbital. The form on the left, however, is something that can be written by hand on a whiteboard or in a homework set. I will use both forms in these class notes, but in class I will mostly use the 2D form on the left.



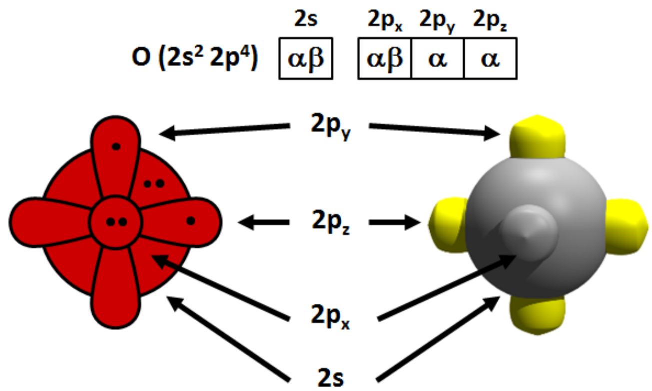
As drawn here, both of these diagrams are empty, containing no electrons yet. Different conventions are used in the two cases to indicate orbital occupations. For the 2D form, we will place dots in the orbitals to indicate the occupation. The dots should always be placed next to each other, rather than one in each lobe of a p orbital. Remember that the dots don't indicate the positions of the electrons (which is precluded by the Heisenberg principle), only the occupations.

The conventions we will use for occupations are shown here:

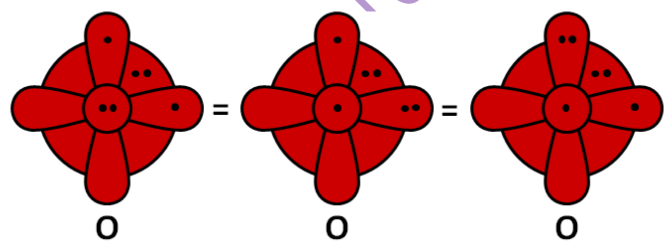


H and He are shown in both forms. For the 2D form on the left, H has one electron in its 1s orbital as indicated by one dot. It can be either spin α or β—the dot doesn't tell us which. The 1s^2 pair for He is denoted with two dots, which always indicates an αβ pair since two electrons with the same spin can never be together in an orbital. The third image is forbidden by the Pauli principle, since we can never put three electrons in the same orbital. For the 3D representations on the right side of the figure, a somewhat transparent, pale green in color is used to indicate an empty orbital (as noted above). Single occupation is indicated with yellow (spin α) or blue (spin β), such as in the case of the 1s^1 orbital on H. Finally, double occupation is denoted with opaque gray, as in the case of the 1s^2 pair on He.

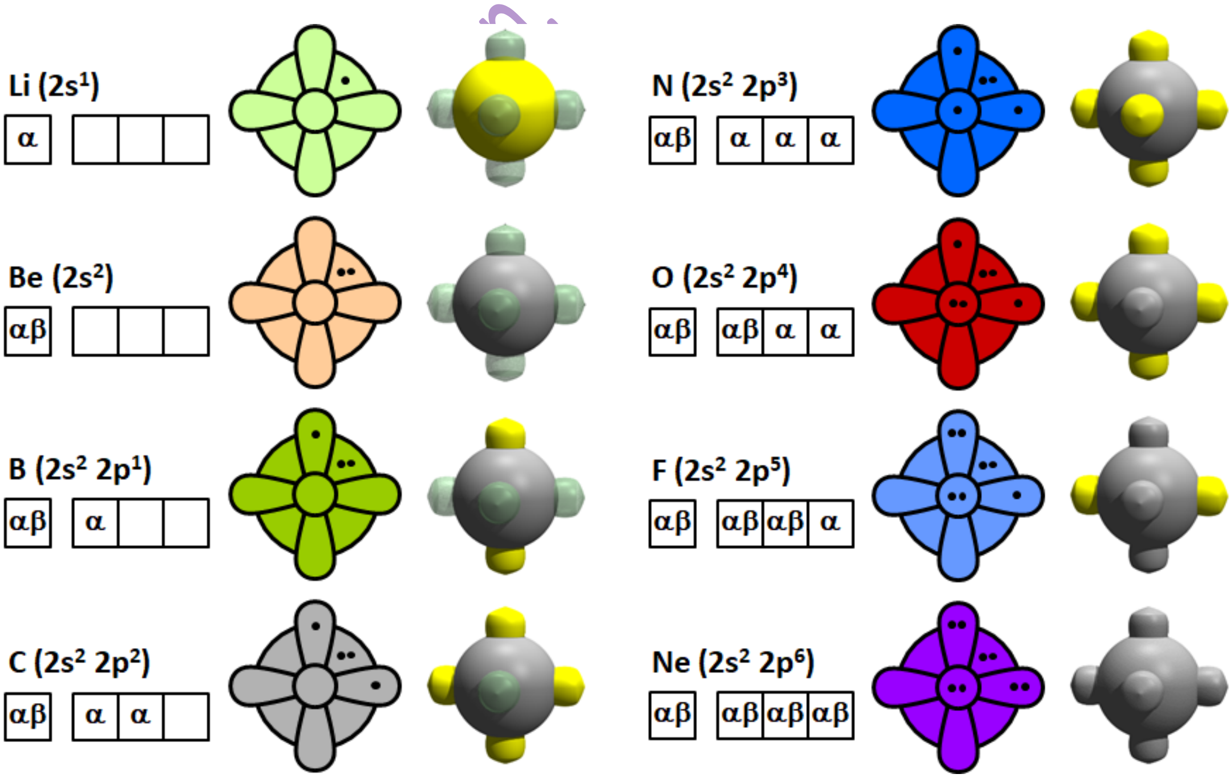
Now let's look at something more complex, the O atom. It has six valence electrons (which is all we will include). The 2s^2 pair is denoted with a pair of dots in the larger, partially obscured circle in the 2D form and by a solid, opaque gray sphere in the 3D form. The in-plane 2p orbitals are each singly occupied, while the out-of-plane 2p orbital is doubly occupied. In the 2D form there are 1 or 2 dots in the orbitals, while we use yellow for the singly occupied orbitals in the 3D form and gray for the doubly occupied ones. They barely peek out from the $2s^2$ pair.



There is nothing special about the occupations shown. Depending on what we are doing with molecules, we could represent O in any of three equivalent ways shown here.

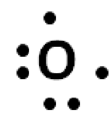


Here is the entire set of atoms from Li–Ne in their ground states:

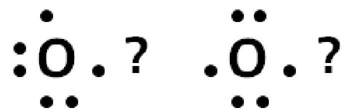


The colors selected for the 2D forms are arbitrary (although in some cases they're similar to color codes used in molecular model kits or graphics programs). Even though all of the 2p orbitals are unoccupied in Li and Be atom, they are shown. In some cases, we may omit the empty 2p orbitals or may not include the $2s^2$ pair. But we will find that these orbitals have critical importance later in the course, so it is important to include them at this point.

B. Configuration diagrams are superior to Lewis diagrams.



You are likely familiar with Lewis (dot) diagrams from previous courses. They are less useful than configuration diagrams because they convey less information. Consider the standard Lewis diagram for O, which shows its six valence electrons as dots arrayed on the four sides of the "O". While the presence of two pairs of dots and two single dots is consistent with the $2s^2\ 2p^4$ αβαβαα triplet configuration of the oxygen atom, critical information has been discarded. The pairs are not labeled, and the single electrons are placed by happenstance on adjacent sides. We could have placed them on opposite sides just as easily.



We will find that the new representations of the atoms provide an excellent starting point for anticipating molecular structures.

Bonus Material

The Chinese characters on the first page were not chosen randomly. They represent, from top to bottom, *atom*, *molecule*, *electron*, and *orbital*. They were taken from a paper entitled "Learning Common Chinese Chemical Terms and Characters" by H.-Y. Chao and D. G. Churchill published in *Journal of Chemical Education*. Click **here** to access the entire article (https://doi.org/10.1021/ed085p1210).

In addition, the famous Nazca lines in Peru, which are often miles across, are examples of **geoglyphs** (https://en.wikipedia.org/wiki/Nazca_Lines).