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Technical note

Writing Electron Configuration: An Algorithmic Approach

Shahrokh Ghaffari*, **Shadi Abu-Baker**

Chemistry Department, Ohio University Zanesville, Zanesville, United States

Abstract The goal of the method presented in this paper is introducing students to a simple procedure to arrive at electron configuration and discover its relevance to the Periodic Table. Once that is accomplished, more complicated configuration can be introduced. Writing an electron configuration or electron diagram is an essential topic covered in all introductory chemistry courses. This requirement often proves challenging for certain students. This procedure employs the periodic table as the first step in a multi-step approach that progressively advances students toward the development of an electron diagram. This method is designed specifically for students with little to no background in chemistry. This method can be used both as lecture supplement or a laboratory experiment.

Keywords Electron Diagram, General Chemistry, Laboratory Experiment, Alogrithms

1. Introduction

To demonstrate the electron configuration of the ground state of atoms, a number of methods, diagrams, and analogies have been presented [1-12]. Although, there are exceptions in the arrangement of electrons in different energy and sub energy levels, in most cases this can be explained by a simple rule. In most cases, students memorize one of the different versions of the Aufbau Principle of the distribution of electrons in different orbitals following Hund's Rule and the Pauli Exclusion Principle. Using quantum mechanics to calculate values of various quantum numbers to give the electron distribution of an atom is challenging and beyond the grasp of students with little or no chemistry background.

2. Step I

This step consists of five parts;

1. Figure out the number of energy levels that have electrons

   The number of energy levels = row number
   For example, since all elements from K (potassium) to Kr (Krypton) are in row number 4, they all have 4 energy levels.
   Write down the maximum possible number of electrons for each energy level using "2xn2".

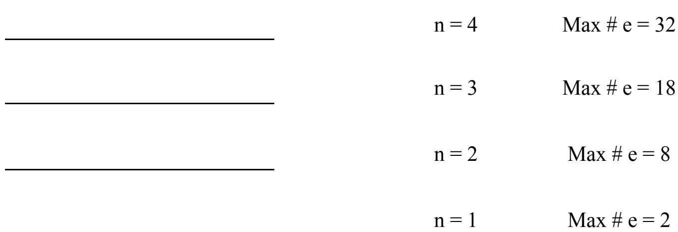

Figure 1. Energy Levels with Maximum Number of Electrons

* Corresponding author:
ghaffari@ohio.edu (Shahrokh Ghaffari)
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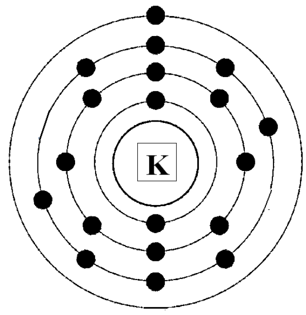
2. First add electrons to the last energy level that is determined in part 1.
   a. For the main group elements add a number of electrons equal to the column number (numbered 1 to 8)
   b. For transitional metal add 2 electrons, except Cr and Cu in row number 4 and Mo and Ag in row number 5 is 1.
3. At this point, start distributing electrons in the lower energy levels, starting from n = 1 until either have their maximum or no more electrons left. That can be presented also as Figures 2(b).

1	n = 4	Max # e = 32
8	n = 3	Max # e = 18
8	n = 2	Max # e = 8
2	n = 1	Max # e = 2

(a)



(b)

Figure 2. Potassium, K (19)

2	n = 4	Max # e = 32
14	n = 3	Max # e = 18
8	n = 2	Max # e = 8
2	n = 1	Max # e = 2

Figure 3. Iron, Fe (26)

1	n = 4	Max # e = 32
13	n = 3	Max # e = 18
8	n = 2	Max # e = 8
2	n = 1	Max # e = 2

Figure 4. Chromium, Cr (24)

3. Step II

1. The next level boxes are added to each energy level with a maximum number of electrons going in each one. The number in each box indicates the possible maximum number of electrons in each. To assign the possible number of electrons in each box start with “2” in the first box on the left. For the next box “4” is added (2 + 4 = 6). The plus “4” rule is followed to assigned the number of possible electrons in the rest of the boxes on the same energy level.

2	6	10	14	n = 4	Max # e = 32
2	6	10		n = 3	Max # e = 18
2	6			n = 2	Max # e = 8
2				n = 1	Max # e = 2

Figure 5. Total Electron Distribution in Orbitals

2. Boxes with 2 electrons are labeled “s”, boxes with 6 electrons “p”, boxes with 10 electrons “d”, boxes with 14 electrons “f”. The boxes represent orbital sublevels.

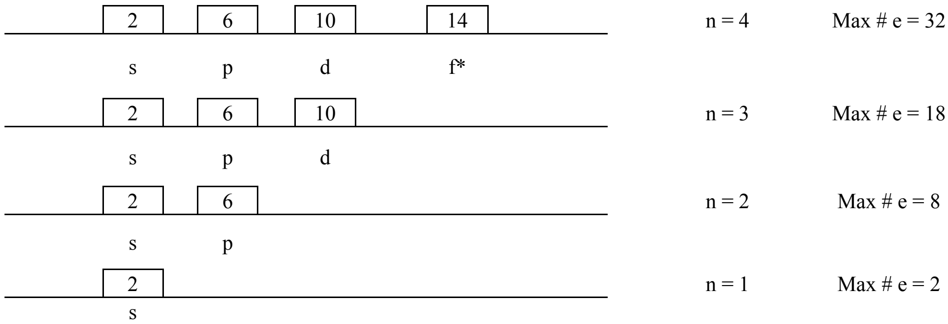


Figure 6. Labeling Orbitals

*. Since students at the intended level are not introduced to any application that required knowledge of “f” orbitals this paper is not covering elements after atomic number 56. The “f” orbitals are filled only after element 66.

3. For each energy level, start from left to right and distribute the electrons in boxes using the calculated number of electrons for each energy level of the atom in Step I.

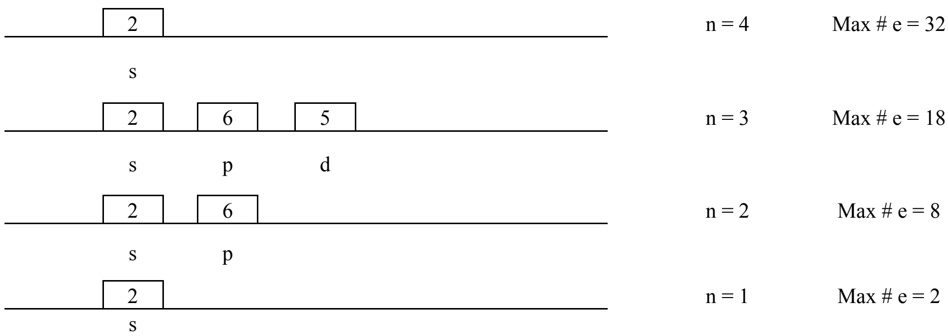


Figure 7. Manganese, Mn (25)

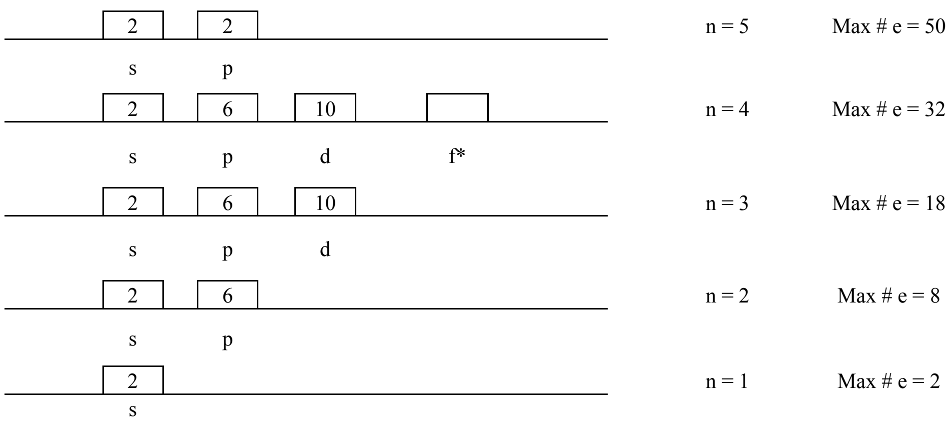


Figure 8. Tin, Sn (50)

*. Since “f” orbitals are only filled after element 66 they are left empty

4. Step III

1. At this point the idea of sub-boxes is introduced that each can hold not more than two electrons. Starting with “s” there is only one orbital. As we move to the next “p” increases by +2-- that is 3 orbitals--and for “d” there are 2 more and so on.

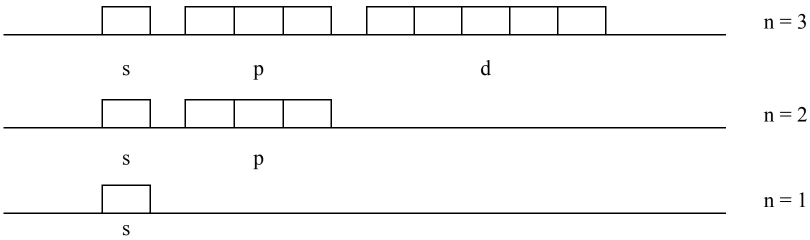


Figure 9. Splitting Orbitals

2. In this step, boxes are rearranged in order of increasing energies of sub-levels.

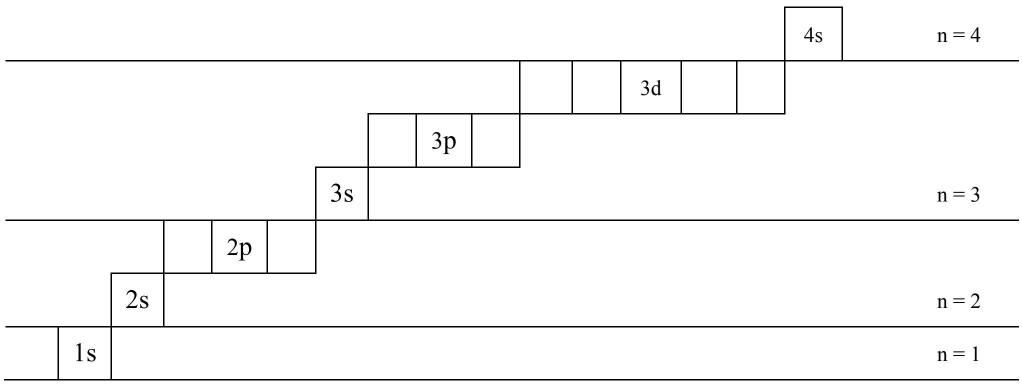


Figure 10. Orbital Energy Level

3. At this point Hund's Rule and Pauli Exclusion Principle are introduced and arrows are used to represent electrons and indicate the direction of electron spin in each orbital.

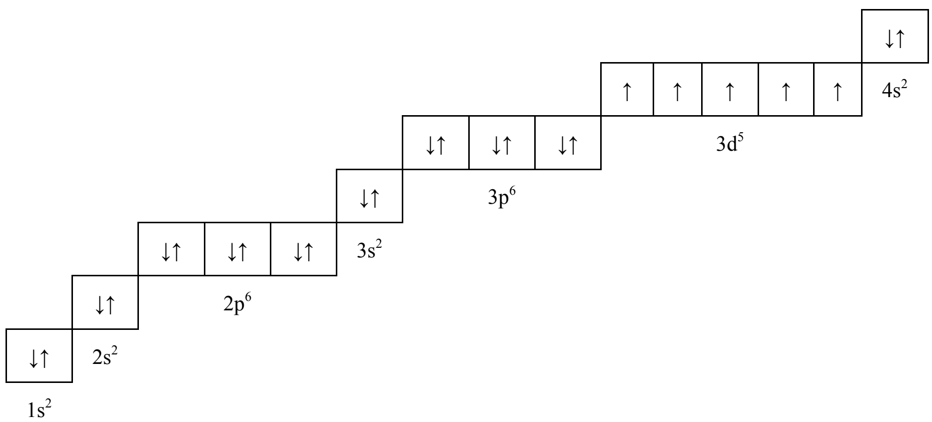


Figure 11. Manganese, Mn (25)

4. Finally the electron configuration is presented in the following form.

$$Mn:\ \underset{1s^2}{\uparrow\downarrow},\ \underset{2s^2}{\uparrow\downarrow},\ \underset{2p^6}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow},\ \underset{3s^2}{\uparrow\downarrow},\ \underset{3p^6}{\uparrow\downarrow\ \uparrow\downarrow\ \uparrow\downarrow},\ \underset{3d^5}{\uparrow\ \uparrow\ \uparrow\ \uparrow\ \uparrow},\ \underset{4s^2}{\uparrow\downarrow}$$

Figure 12. Manganese, Mn (25)

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