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Teaching Atomic Structure: Madelung's and Hund's Rules in One Chart

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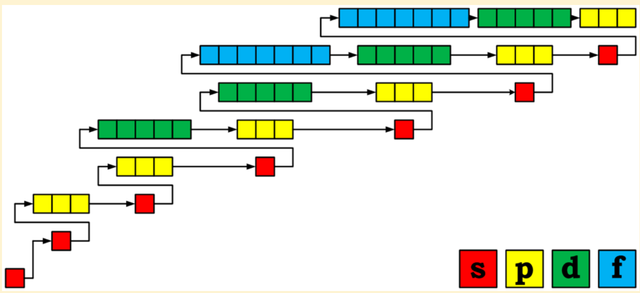
Supporting Information

ABSTRACT: A diagram that represents electron levels and sublevels with the corresponding values of quantum numbers has been designed. The main purpose of the diagram is the explanation of the atomic structure to the students according to Hund's rule and especially Madelung's rule. The diagram represents a specific arrangement of all sublevels' orbital diagrams in order to enhance the understanding of said rules.



KEYWORDS: *High School/Introductory Chemistry, Physical Chemistry, Textbooks/Reference Books, Atomic Properties/Structure*

Successful methods have been developed for teaching electron configurations, especially the order for filling the atomic orbitals with electrons.[1−5] However, a diagram that would display both the order for filling the orbitals and electron occupancy of the orbitals has not been reported. Electron occupancy of the orbitals is usually explained with the help of orbital diagrams, which play a particularly important role in teaching electron distribution in atoms and are further used in description of chemical bonding. Design of a diagram that would combine Madelung's and Hund's rules in one chart might further advance the educational process.

■ DESCRIPTION

In Figure 1, seven columns represent energy levels. Within a column, levels are divided into energy sublevels. An arithmetic progression is observed: the first level contains one sublevel, the second level contains two sublevels, the third level contains three sublevels, etc. Sublevels consist of an odd number of atomic orbitals (1, 3, 5, 7, 9, 11, 13, etc.), and each cell stands for one atomic orbital.

The top row shows the values of the principal quantum number n (every positive integer) which determine the level. The values of the orbital quantum number l (every integer from 0 to $n - 1$) are not shown but encoded into the sublevel symbols (1s, 2p, 3d, etc.), and they determine the sublevel within the level, i.e.,

$l = 0 \Rightarrow$ s-sublevel

$l = 1 \Rightarrow$ p-sublevel

$l = 2 \Rightarrow$ d-sublevel

$l = 3 \Rightarrow$ f-sublevel

and so on in alphabetical order (g, h, i, etc.). The second top row shows the values of the magnetic quantum number m (every integer from $+l$ to $-l$) which determine the atomic orbital within the sublevel; the sublevels within a level are arranged symmetrically according to equal values of m. Consequently, a set of quantum numbers n, l, m step by step determines the atomic orbital that contains the observed electron.[6]

The value of $n + l$ describes the relative energy of sublevels. All sublevels are arranged into horizontal lines with equal value of $n + l$ given in the left column to explain Madelung's rule: sublevels with the lowest value of $n + l$ are filled in the first place; among a number of sublevels with equal value of $n + l$, the one with the lowest value of n is filled in the first place. Therefore, with the suggested diagram, the sublevels are filled row by row from bottom to top, and within rows the sublevels are filled from left to right. The order for filling the sublevels with electrons according to Madelung's rule is displayed in Figure 2.

The order for filling the sublevels with electrons is justified by the overlap of energy levels with the increase of the principal quantum number.[7] As n increases, there is a switch in relative energy of the sublevels, for example, 4s is lower in energy than 3d.

In Figure 1 (for a high-definition printable version of the diagram see Supporting Information), sublevels with $n + l > 8$ are set off in dashed lines as such sublevels are not occupied in any chemical element's atom on Earth (according to Madelung's rule, 7p atomic orbital is followed by 8s, but that would correspond to the first chemical element in the eighth period which is yet to be discovered, so the diagram does not show the eighth level). These sublevels, though, are not omitted in order to highlight the above-mentioned arithmetic progression and provide the most proper understanding of the

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J. Chem. Educ. XXXX, XXX, XXX−XXX

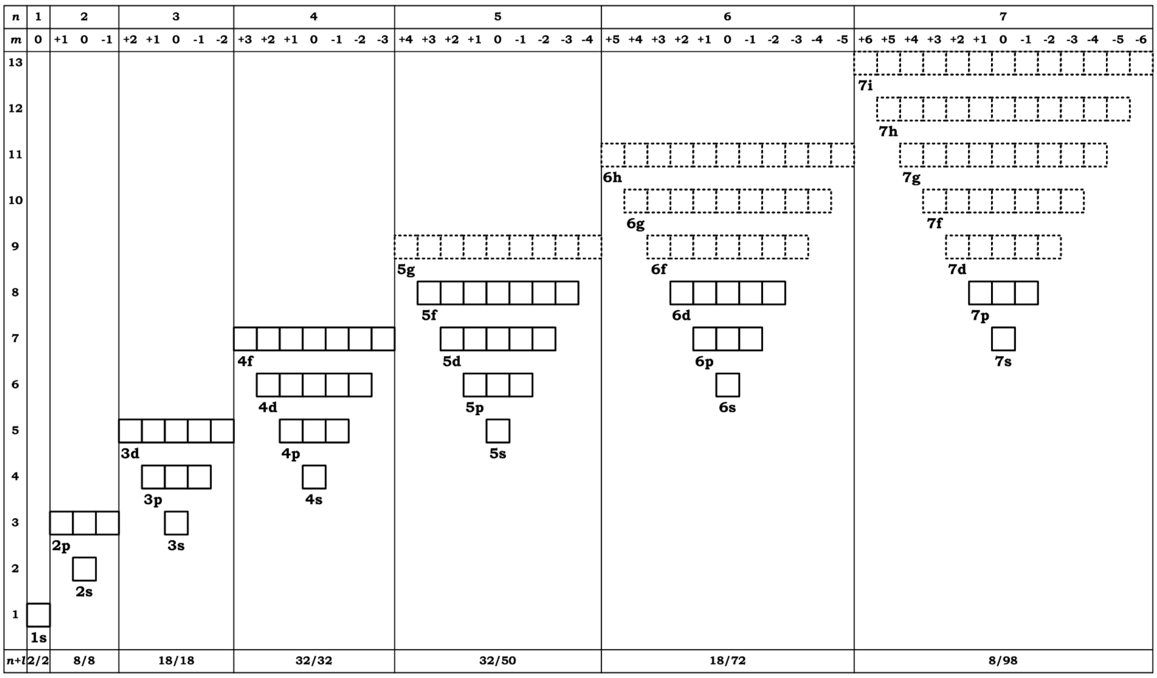

Figure 1. Suggested diagram.

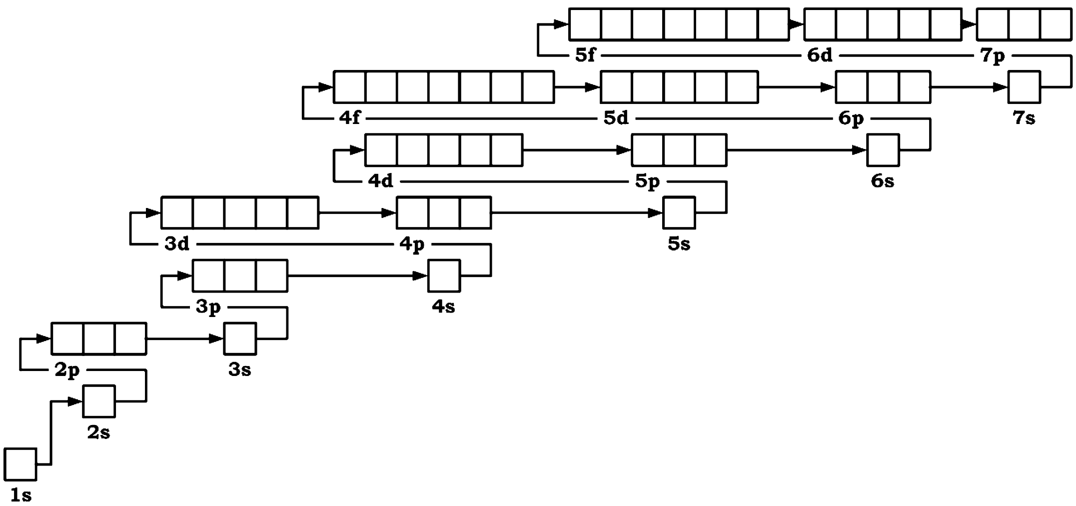

Figure 2. Order for filling the sublevels with electrons according to Madelung's rule.

theorized chemical elements' electron configurations. The bottom row shows the actual number of electrons within a level against the maximum possible number $2n^2$. The actual number becomes less than the maximum possible number starting with the fifth level due to sublevels like 5g bearing no electrons.

■ UTILIZATION

The suggested diagram allows to display the distribution of electrons in any chemical element's atom in both ground and excited states. A good example is the excited state of a phosphorus's atom (Figure 3).

Phosphorus's atom ground state condensed electron configuration is $[_{10}\mathrm{Ne}]3s^23p^3$, which is convenient to display with the suggested diagram. Hund's rule is applied for 3p sublevel: when orbitals of equal energy are filled, the electrons remain unpaired as long as possible to minimize electron–electron repulsion; hence, the atom is most stable.[7,8]

In its excited state, one electron leaves the 3s sublevel and occupies an atomic orbital of the 3d sublevel, which results in phosphorus's electron configuration $[_{10}\mathrm{Ne}]3s^13p^33d^1$. James E. House suggests that for convenience the atomic orbital with the highest value of m is filled in the first place.[8] Therefore, with the suggested diagram the atomic orbitals of a sublevel are filled with electrons from left to right. The diagram gives the opportunity to perform a comparative analysis of chemical elements' electron configurations in ground or excited states by differentiating them with color.

■ ADVANTAGES AND LIMITATIONS

With the help of the suggested diagram, the students learn the values of quantum numbers n, l, and m and understand how they determine the levels, the sublevels, and the atomic orbitals,

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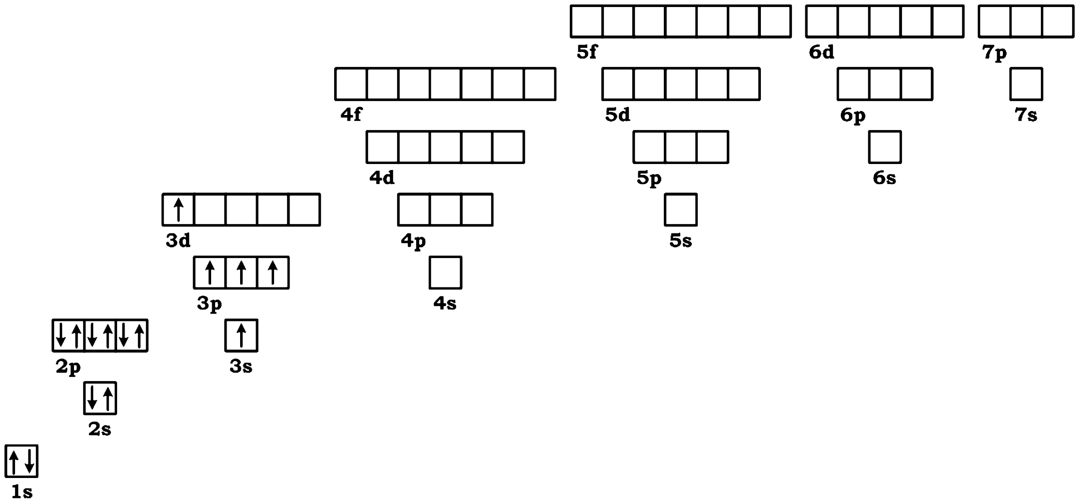

Figure 3. Excited state of a phosphorus's atom.

respectively. The students understand the distribution of electrons in an atom as they get a visual representation of Madelung's and Hund's rules in one chart. Teachers are encouraged to print the diagram and distribute it among students during classes. The chart is not an atomic energy level diagram and is designed solely for educational purposes.

■ ASSOCIATED CONTENT

Ⓢ Supporting Information

A high-definition printable version of the diagram. This material is available via the Internet at http://pubs.acs.org.

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Notes

The authors declare no competing financial interest.

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