B.Sc. (Honours) Part-I
Paper-IB

Topic: Hunds Rule of Maximum Multiplicity

UG

Subject-Chemistry

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Hund's rule

Hunds Rule of Maximum Multiplicity:

Hunds Rule of Maximum Multiplicity rule states that for a given electron configuration, the term with maximum multiplicity falls lowest in energy. According to this rule electron pairing in p, d and f orbitals cannot occur until each orbital of a given subshell contains one electron each or is singly occupied.

Hund's rule states that:

1. Every orbital in a sublevel is singly occupied before any orbital is doubly occupied.
2. All of the electrons in singly occupied orbitals have the same spin (to maximize total spin).

When assigning electrons to orbitals, an electron first seeks to fill all the orbitals with similar energy (also referred to as degenerate orbitals) before pairing with another electron in a half-filled orbital. Atoms at ground states tend to have as many unpaired electrons as possible. In visualizing this process, consider how electrons exhibit the same behavior as the same poles on a magnet would if they came into contact; as the negatively charged electrons fill orbitals, they first try to get as far as possible from each other before having to pair up.

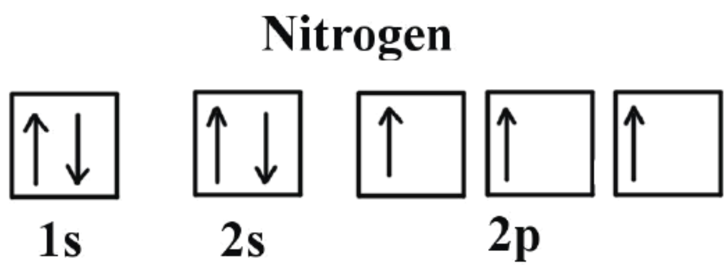
Explanation of Hund's Rule

The electrons enter an empty orbital before pairing up. The electrons repel each other as they are negatively charged. The electrons do not share orbitals to reduce repulsion.

When we consider the second rule, the spins of unpaired electrons in singly occupied orbitals are the same. The initial electrons spin in the sub-level decides what the spin of the other electrons would be. For instance, a carbon atom's electron configuration would be $1s^22s^22p^2$. The same orbital will be occupied by the two 2s electrons although different orbitals will be occupied by the two 2p electrons in reference to Hund's rule.

Example 1: Nitrogen Atoms

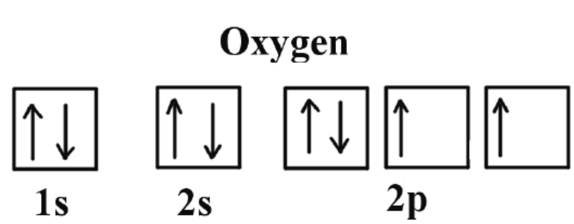
Consider the correct electron configuration of the nitrogen (Z = 7) atom: $1s^2\ 2s^2\ 2p^3$



The p orbitals are half-filled; there are three electrons and three p orbitals. This is because the three electrons in the 2p subshell will fill all the empty orbitals first before pairing with electrons in them.

Example 2: Oxygen Atoms

Oxygen (Z = 8) atom, the element after nitrogen in the same period; its electron configuration is: $1s^2\ 2s^2\ 2p^4$



Example 3: Carbon Atoms

Take the electron configuration for carbon: 2 electrons will pair up in the 1s orbital, 2 electrons pair up in the 2s orbital, and the remaining 2 electrons will be placed into the 2p orbitals. The correct orbital diagram, obeying Hund's Rule, will note the two 2p electrons to be unpaired in two of the three available orbitals, both with "spin-up." Since electrons always occupy an empty orbital before they fill up, it would be incorrect to draw the two 2p electrons in the same orbital, leaving open orbitals unfilled.