HYPERCONJUGATION

Hyperconjugation Effect (H-Effect)

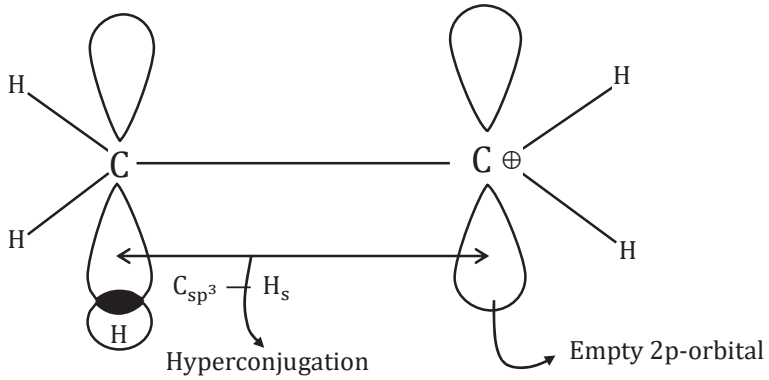
Complete transfer of e– of C–H σ bond towards π bond or positive charge or free electron is called as H-effect (permanent effect). It is also called as No bond resonance (given by Nathen and Baker).

Applications of Hyperconjugation

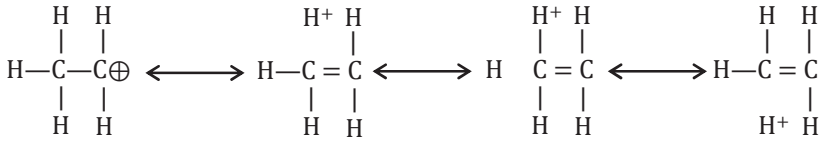
Relative Stability of Carbocation

hyperconjugation can happen in organic compounds when there's a positively charged carbon atom with an empty p-orbital.

Let's look at $CH_2CH_2^{\oplus}$ (ethyl cation). In this case, one of the bonds between carbon and hydrogen in the methyl group can line up with the empty p-orbital. The electrons that make up this bond can then spread out into the empty p-orbital. So, in this situation, hyperconjugation occurs because a C—H bond (formed by sp^3-s overlap) partially overlaps with the empty p-orbital of a nearby positively charged carbon atom.



We can illustrate hyperconjugation in the ethyl carbocation like this:



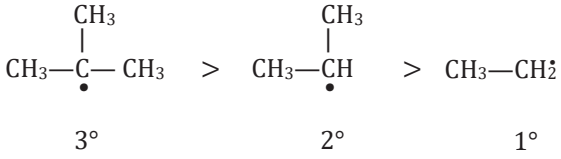
In simple terms, when there are more alkyl groups connected to the positively charged carbon atom, there is a stronger hyperconjugation interaction. This leads to increased stabilization of the cation. Therefore, the carbocation becomes less stable when there are fewer alkyl groups.

$$(CH_3)_3\,C^+ > (CH_3)_2\,CH^+ > CH_3\,CH_2^+ > CH_3^+$$

Relative Stability of Free Radical

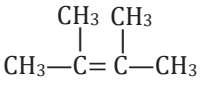
The stability of free radicals follows the same order as carbocations, which is 3° (tertiary) > 2° (secondary) > 1° (primary). This stability order can be easily understood through hyperconjugation. When there are more alkyl groups connected to the carbon carrying the unpaired electron, the electron is spread out more, making the alkyl free radical more stable.

Therefore,

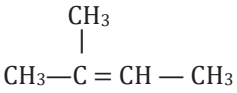


Relative Stability of Alkene

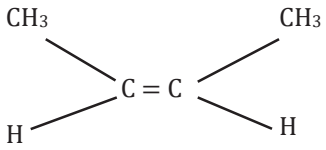
The stability of alkenes is also explained by hyperconjugation. When there are more alkyl groups attached to the carbon atoms forming the double bond, the alkene becomes more stable. Let's look at the following alkenes:



12 α -Hydrogen



9 α -Hydrogen



9 α -Hydrogen

Number of α – hydrogen = Number of Hyperconjugation structure

Because the more hyperconjugation structures there are, the more stable the alkene becomes, the relative stability of these alkenes can be described as follows:

$$1 > 2 > 3 > 4$$