HYPERCONJUGATION

Julien Racine*[1] and Stéphane Humbel*[1]

[1]ctom – Université Paul Cézanne - Aix-Marseille III – France

Résumé

Carbocations can appear in transient species, for instance in nucleophilic substitutions, in elimination reactions, and various rearrangements. Hyperconjugation (or conjugation) can then stabilize the cationic character and form a partial π bond. We computed the effect of the electronic delocalization in strained substituents of a -CH2+ carbocation part. We found very large hyperconjugation effects, sometimes more than 80 kcal/mol, hence much larger than typical conjugation effects (56 kcal/mol for the allyl cation).

Mots-Clés: Carbocation, hyperconjugation, BLW

*Intervenant