HYPERCONJUGATION

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Résumé

Carbocations can appear in transient species, for instance in nucleophilic substi-
tutions, in elimination reactions, and various rearrangements. Hyperconjuga-
tion (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

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