CONFORMATIONS OF SUBSTITUTED ACETYLENES: 3-HEPTYNE, (CH_3CH_2-CC-$CH_2CH_2CH_3$) IS NEARLY ECLIPSED

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Alkanes have staggered rather than eclipsed configurations about C-C bonds. Some theorists make the case that the dominant effect is hyperconjugative stabilization of vicinal C-H bonds in the anti configuration rather than steric repulsion. Butane has gauche and anti conformations consistent with staggered configurations. However, when the two ethyl groups of butane are separated by an acetylene CC triple bond (3-hexyne), they become syn eclipsed[a] suggesting that the putative symmetry control of hyperconjugation is lost in this extended form and that the steric repulsion of vicinal substituents when they are separated by less than the sums of their van der Waals radii as in butane becomes a gentle dispersive attraction at larger separations as in 3-hexyne. 3-Heptyne (ethyl propyl acetylene) is the extended analog of pentane. We have assigned the microwave spectrum of the conformer with the propyl group in a gauche configuration: A = 4826.475(2), B = 1165.0309(2), and C = 989.5941(2) MHz. The terminal ethyl and propyl groups are approximately eclipsed. Search for the spectrum of the expected conformer with the propyl group in an anti configuration continues.

[a] R. K. Bohn, J. Phys. Chem. A. 108, 6814 (2004).