3-HEXYNE, (CH_3CH_2-CC-CH_2CH_3), HAS C_{2v} SYMMETRY

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Ethane has a staggered equilibrium geometry with an internal rotation barrier of about 3 kcal/mol. Most chemists accept that that geometry is the result of steric repulsion among the H atoms but Lionel Goodman and others have made a strong case that the dominant effect is hyperconjugative stabilization of the anti orientation of vicinal C-H bonds, i.e., a symmetry controlled effect. When the two methyl groups are separated by a CC triple bond (CH_3-CC-CH_3), the torsional barrier drops to only 0.016 kcal/mol and the stable configuration is unknown. A corollary of ethane's stable geometry is that butane ($CH_3CH_2CH_2CH_3$) has stable gauche and anti conformations consistent with ethane's staggered geometry. We have observed and assigned the b-type microwave rotational spectrum of 3-hexyne, butane with a CC triple bond inserted between the two ethyl groups. The rotational constants are A = 9410.842(7) MHz, B = 1407.795(2) MHz, and C = 1269.727(2) MHz and several centrifugal distortion constants have been determined. The structure has C_{2v} symmetry for several reasons. The c second moment is 7.31 uA^2 consistent with a planar heavy atom structure, no tunneling splittings are observed indicating a single torsional minimum (therefore, not C_2), and it has a microwave spectrum and therefore a permanent dipole moment (not C_{2h}). The result suggests that the symmetry argument relevant to the stable conformation of ethane does not carry over to this elongated analogue of ethane.