MICROWAVE STUDY OF 2-METHYL-1-HEXENE-3-YNE [CH_3CH_2-CC-C(=CH_2)CH_3]: GROUND STATE AND TORSIONALLY EXCITED STATE

JOSEPH YEAGER, *Dept. of Chemistry, Centre College, Danville, KY 40422*; ROBERT K. BOHN, *Dept. of Chemistry, Univ. of Connecticut, Storrs, CT 06269-3060*.

Alkanes have staggered rather than eclipsed configurations about C-C single bonds. In contrast, alkenes exist in syn (C-C-C=C dihedral angle 0 deg) and skew(H-C-C=C dihedral angle 0 deg) conformations about the =C-C bond. When alkanes are elongated by inserting a CC triple bond between alkyl fragments, the conformation relating the alkyl fragments about the acetylene axis is no longer staggered but syn-eclipsed. This has been demonstrated for the elongated forms of butane (diethyl acetylene) and pentane (ethyl propyl acetylene). The title compound is the elongated form of 2-methyl-1-butene [$CH_3CH_2C(=CH_2)CH_3$] which probably exists in syn and skew forms. (2-Methyl-1-butene has not been studied.) The microwave spectrum of the title compound has been observed in a pulsed-jet Fourier Transform spectrometer and assigned. Two species are present. One has a planar heavy atom structure with the C-C-(CC)-C=C dihedral angle 180 deg and the other we interpret to be a low-lying (within a few cm^{-1}) torsionally excited state. Rotational constants for the ground state and excited state are 6530.95(35), 1116.2016(6), and 9742.2051(5) MHz and 6758.9(22), 1092.041(6), and 971.510(7) MHz, respectively. The latter spectrum is fit to an rmsd of 71 kHz indicating that we have not yet found a Hamiltonian that models the large amplitude torsion well.