MICROWAVE STUDIES OF TWO CONFORMERS OF 6-METHYL-3-HEPTYNE AND THREE OF 2-METHYLPENTANE

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The equilibrium torsional angle between two alkyl substituents connected by a C≡C linkage is determined by delicate interactions between the groups. 6-Methyl-3-heptyne (ethyl isobutyl acetylene,) displays rotational microwave spectra of two conformers, C_s and C_1 symmetry, which arrange the opposing alkyl groups syn-eclipsed or nearly so. The dominant interaction determining the dihedral angle about the acetylene axis is the small dispersion attraction between the ethyl and isobutyl groups. 2-Methylpentane, 6-methyl-3-heptyne without C≡C, has three characterized conformers. The alkane has more conformations than the alkyne because the C2-C3 bond has a substantial ethane-like barrier supporting gauche and anti conformations while the alkyne's C2-(C≡C)-C5 tiny torsional barrier has only a single minimum.

Rotational constants for the two conformers of 6-methyl-3-heptyne are 3282.9197(6), 942.43143(20), and 886.33450(16) MHz and 4603.7990(7), 798.12154(13), and 713.87656(11) MHz, respectively. Rotational constants for the three conformers of 2-methypentane are 5820.1248(5), 1848.9706(3), and 1656.7897(4) MHz; 6615.4521(10), 1713.06566(20), and 1473.09913(11) MHz; and 5501.9431(11), 1980.37687(20), and 1789.41065(20) MHz, respectively. Each spectrum is fit to an rmsd of 3 kHz or less.