CONFORMATIONS AND BARRIERS ABOUT TRIPLE BONDS: ISOPROPYL PHENYL ACETYLENE

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The triple bond in acetylene is cylindrically symmetrical. Therefore, the internal rotation barrier about that axis in substituted acetylenes is very small, affected only by long range interactions between the remote substituents. In the title compound, the van der Waals' interactions between the isopropyl and phenyl groups occur in the weakly attractive range of these forces, determine the stable conformation, and are the dominant factors in the torsional potential. Microwave rotational spectra of phenyl isopropyl acetylene ($C_6H_5CCCH(CH_3)_2$, 3-methy-1-phenyl-1-butyne) have been observed at rotational temperatures near 1 K on a pulsed-jet Fourier transform microwave spectrometer. Measurements have been taken in the range 6 to 13 GHz. Many of the rotational transitions display tunneling splittings of about a MHz due to the 2-fold internal rotation barrier about the acetylene -CC- axis. Preliminary values of the rotational constants for the lower rotational frequency torsional state are A = 3310(1),B = 447.368(6), and C = 402.976(6) MHz, and for the higher rotational frequency torsional state are A = 3221(1), B = 447.41(2), and 403.00(2) MHz. The torsional energy minimum occurs with the methyls of the isopropyl group lying close to the plane of the benzene ring on one side of it. In contrast, in isopropyl benzene, the analogous molecule with the acetylene -CC- spacer removed, the torsional energy minimum occurs with the methyls forced out of the benzene plane and located on opposite sides of it. Analysis of the tunneling splittings is continuing.