CONFORMATIONS AND INTERNAL ROTATION IN PHENYL ETHYL ACETYLENE

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Microwave rotational spectra of phenyl ethyl acetylene ($C_6H_5CCCH_2CH_3$, 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 5 to 8.7 GHz. Many of the rotational transitions display tunneling splittings of several MHz due to the 2-fold internal rotation barrier about the acetylene -CC- axis. Preliminary values of the B and C rotational constants for the ground and first excited torsional states are B = 557.3169(3), 556.6456(11) and C = 500.7120(4), 500.8820(13), respectively. Since only a-type transitions have been assigned so far, the A constant is not well determined. The stable conformation appears to have a planar-heavy-atom structure which contrasts with the orthogonal orientation of the phenyl and ethyl groups found in ethyl benzene, ethyl phenyl acetylene with the -CC- spacer removed.