

THE MILLIMETER-WAVE ROTATIONAL SPECTRUM OF PHENYLACETYLENE

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The rotational spectrum of phenylacetylene, $\text{C}_6\text{H}_5-\text{C}\equiv\text{C}-\text{H}$, has hitherto only been studied in the centimeter-wave region, at room-temperature,^a and in supersonic expansion.^b There appears to be continuing astrophysical interest in polar species closely related to benzene and we decided to extend the knowledge of the laboratory spectrum of phenylacetylene up to the submillimeter-wave region. We report extensive measurements of the room-temperature spectrum at frequencies from 90 to 340 GHz. Precise spectroscopic constants are determined for the ground state, and the two lowest excited vibrational states: $\nu_{24} = 1$ and $\nu_{36} = 1$.

The two excited states belong to the out-of-plane and the in-plane $\text{C}-\text{C}\equiv\text{C}$ bending modes, and are very strongly coupled by an a -axis Coriolis interaction. It was, nevertheless, possible to successfully fit the measured transitions with a minimal number of interaction constants. The present results from rotational spectroscopy are compared with previous normal mode analyses for phenylacetylene and with additional anharmonic force field calculations carried out in this work.

^aA.P.Cox, I.C.Ewart, W.M.Stigliani, *J. Chem. Soc. Farad. Trans II* **71**, 504-514 (1975).

^bH.Dreizler, H.D.Rudolph, B.Hartke, *J. Mol. Struct.*, **698**, 1-24 (2004).