

MICROWAVE SPECTRUM AND STRUCTURE OF PHENYLACETYLENE...METHANOL COMPLEX

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Phenylacetylene (PhAc) is a multifunctional molecule and has been termed a “Hydrogen Bonding Chameleon”^a. In 2008, Patwari and co-workers studied complexes of PhAc with various molecules, including H₂O and CH₃OH, by the IR-UV double resonance spectroscopic technique^b. This study found that H₂O donates the H-bond to the acetylenic π -system, whereas CH₃OH donates the H-bond to the phenyl π -system. Recently, Suhm’s group used FTIR spectroscopy of supersonic jet expansions to study PhAc with H₂O and CH₃OH and observed that both H₂O and CH₃OH donate H-bond to the acetylenic π -system^c. The acetylenic preference in the PhAc...H₂O complex has already been confirmed by rotational spectroscopy^d. In this work, the rotational spectrum of PhAc...CH₃OH complex has been studied. The rotational spectrum of the parent and isotopologues of PhAc...CH₃OH complex was recorded over the 2-8 GHz frequency range using the Chirped Pulse Fourier Transform Microwave (CP-FTMW) Spectrometer at Newcastle University, UK, and from 8-14 GHz using the Pulsed Nozzle Fourier Transform Microwave Spectrometer (PN-FTMW) at IISc Bangalore, India. The structure where CH₃OH donates the H-bond to the acetylenic π -system and CH₃OH accepts a weak H-bond through the ortho hydrogen of the PhAc was observed. The rotational transitions were split, indicating the internal motion of the CH₃ group in CH₃OH. The observed global minimum structure has been compared with several CH₃OH-containing complexes to understand the internal rotation of the CH₃ group and its effect on V_3 barrier height.

^aMaity, S., Guin, M., Singh, P. C., & Patwari, G. N. (2011). *ChemPhysChem*, 12(1), 26-46.

^bSingh, P. C., & Patwari, G. N. (2008). *The Journal of Physical Chemistry A*, 112(23), 5121-5125

^cKarir, G., Lüttschwager, N. O., & Suhm, M. A. (2019). *Physical Chemistry Chemical Physics*, 21(15), 7831-7840

^dGoswami, M., & Arunan, E. (2011). *Physical Chemistry Chemical Physics*, 13(31), 14153-14162