PURE ROTATIONAL STUDY OF CYANOPHENYLACETYLENE ($C_6H_5C_3N$)

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The reaction of cyano radical with hydrocarbon chains and rings is thought to be important in the formation of complex nitriles, particularly in the formation of polycyclic aromatic hydrocarbons (PAHs). Difficulties in studying these reactions arise from both the plethora of possible product channels, and gaps in our knowledge as to the key species in each pathway. One reaction that has been studied in some detail is cyano radical with phenylacetylene.[a] One of the products identified in this reaction is cyanophenylacetylene (3-Phenyl-2-propynenitrile, $C_6H_5C_3N$), the rotational spectrum of which has not been previously studied. Motivated in part by the recent detection of benzonitrile in the ISM,[b] and the presence of large cyanopolyyne chains there,[c], the pure rotational spectrum of $C_6H_5C_3N$ has been investigated in the 8–18 GHz and 75–220 GHz regions. We will present our results (experimental spectrum and rotational constants), and discuss the various methods we used in fitting the data. The new data now allow a search for this species in the ISM.

[a] Bennett et al., Phys. Chem. Chem. Phys. 12, 8737-8749 (2010)

[b] McGuire et al., Science 359, 202–205 (2018)

[c] Broten et al., ApJL 223, L105-L107 (1978)