# THE 103 - 360 GHZ ROTATIONAL SPECTRUM OF BENZONITRILE, THE FIRST INTERSTELLAR BENZENE DERIVATIVE DETECTED BY RADIOASTRONOMY

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Benzonitrile ($C_7H_5N$, $C_{2v}$, $\mu_a$ = 4.5 D) has recently been detected in the interstellar medium (ISM), specifically in the Taurus Molecular Cloud 1 (TMC-1), using both the technique of composite averages[1−2] and by nine hyperfine-resolved rotational transitions[2] under 50 GHz. While benzonitrile has been thoroughly studied using infrared and cm-wave spectroscopy, no former studies have examined the rotational spectrum above 160 GHz. Herein, we present the analysis and assignment of the mm-wave rotational spectrum of benzonitrile (vibrational ground state) in the 103 – 350 GHz frequency range, which should assist in future astronomical searches. Additionally, we have completed a two-state least-squares fit of the hitherto unreported, Coriolis-coupled dyad of benzonitrile's two lowest frequency vibrational modes: $\nu_{22}$ (141 $cm^{-1}$) and $\nu_{33}$ (163 $cm^{-1}$), resulting in approximately 3000 transitions per state fit to within experimental accuracy. The two-state fit accounts for many resonances between the two states and 11 nominal interstate transitions. As a result, we have determined the energy gap between the vibrational states ($\Delta E_{22,33}$= 19.108187(7) $cm^{-1}$) and the Coriolis coupling value ($\zeta_{22,33}{}^{a}$ = 0.841(5)). The study demonstrates that the lowest energy fundamentals of benzonitrile follow the previously described pattern of this molecular class.

1. Kalenskii, S. V., Possible Detection of Interstellar Benzonitrile. Proceedings of the Russian-Indian workshop on radio astronomy and star formation, October 10-12, 2016 (eds. I. Zinchenko & P. Zemlyanukha), Institute of Applied Physics RAS, p.43-50, 2017. 2. McGuire, B. A.; Burkhardt, A. M.; Kalenskii, S. V.; Shingledecker, C. N.; Remijan, A. J.; Herbst, E.; McCarthy, M. C. Science 2018, 359 (6372), 202-205.