

MILLIMETER-WAVE SPECTRUM OF 2-CYANOPYRIDINE IN ITS GROUND STATE AND THE DYAD OF ITS LOWEST ENERGY VIBRATIONALLY EXCITED STATES, ν_{30} AND ν_{21}

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In this study, we collected the 135-375 GHz rotational spectrum of 2-cyanopyridine, a N-heteroatom analog of the interstellar molecule, benzonitrile. 2-Cyanopyridine's strong dipole moment ($\mu_a = 5.5$ D, $\mu_b = 1.9$ D) and the fact that it is a cyano substituted aromatic molecule make it another attractive species for detection by radioastronomy. The ground state of 2-cyanopyridine was fit to a centrifugally distorted single state model using Kisiel's ASFIT ($N_{lines} \sim 6500$, $\sigma = 0.043$) and primarily includes ${}^bR_{-1,1}$, ${}^aR_{0,1}$, and ${}^bR_{1,1}$ type lines. The two lowest fundamentals, ν_{30} and ν_{21} , display effects of strong Coriolis interactions and require treatment *via* a two-state model. Discreet local resonances with $\Delta K_a = 3$ perturbation have been seen along with the effects of a strong a-type global perturbation. Currently, using Pickett's SPFIT, around 16,000 distinct rotational transitions for these states have been measured, from $K_a = 0$ to 49 and $J'' = 11$ to 146, leading to an experimental energy difference of $\Delta E_{30,21} = 793379.9$ MHz (~ 26.5 cm^{-1} , compared to a 30.6 cm^{-1} B3LYP/6-311+G(2d,p) anharmonic frequency prediction). Six perturbation terms, including G_a, G_b, F_{bc} and the higher order terms, G_a^J, G_b^J, G_b^K , are currently being treated; and those predicted agree to within 10% of the prediction. This presentation will expand on the progress of the two state least squares fit and full results of the millimeter-wave analysis of 2-cyanopyridine.