

ROTATIONAL SPECTROSCOPY OF *SYN* AND *ANTI-CLINAL* PENTA-3,4-DIENENITRILE FROM 130-375 GHz

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Penta-3,4-dienitrile, (P34DN, $\text{H}_2\text{C}=\text{C}=\text{CHCH}_2\text{CN}$), is an intriguing target for detection in the interstellar medium and the atmosphere of Titan because of its structural similarity to known interstellar molecules and because it is a constitutional isomer of the simple aromatic compound, pyridine ($c\text{-C}_5\text{H}_5\text{N}$). P34DN has recently been synthesized in our group and its millimeter-wave spectrum has been collected from $\sim 130\text{-}375$ GHz. Computational studies reveal that P34DN has two stable conformers linked by the internal rotation of the $-\text{CH}_2\text{CN}$ group and separated by <1 kcal/mol. The internal rotation is the lowest fundamental, ν_{27} , in both conformers. Over 800 distinct rotational transitions of the ground vibrational state of the *syn* conformer (C_s , $\mu_a = 1.7$ D, $\mu_b = 3.1$ D, CCSD(T)/cc-pVTZ) have been least-squares fit to a single-state centrifugally distorted rotor model using Kisiel's ASFIT, and analysis of this ground state is ongoing.

The *anti-clinal* conformer of P34DN has C_1 symmetry ($\mu_a = 3.4$ D, $\mu_b = 1.9$ D, $\mu_c = 0.6$ D, CCSD(T)/cc-pVTZ). Rotational transitions for the ground state and the vibrational states ν_{27} , $2\nu_{27}$, $3\nu_{27}$, and $4\nu_{27}$ have been identified. Clear evidence of strong Coriolis coupling between the ground state and ν_{27} ($\sim 52\text{ cm}^{-1}$) has been observed, primarily between $K = 18$ of the ground state and $K = 14$ of the excited state. Coupling is also observed between the $v = 1$ and $v = 2$ of ν_{27} . This presentation will discuss the current analysis of the coupling between the ground state and ν_{27} $v = 1$ and the current status of their coupled least-squares fit using Pickett's SPFIT program.