THE CONFORMER SPECIFIC ROTATIONAL SPECTRUM OF 3-PHENYLPROPIONITRILE UTILIZING STRONG FIELD COHERENCE BREAKING

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The 8-18 GHz conformer specific rotational spectrum of gauche- and anti-3-phenylpropionitrile (C6H5-CH2-CH2-CN) conformers has been recorded using the strong field coherence breaking (SFCB) technique [1] with a modified line picking scheme for multiple selective excitations (MSE). As the recombination product of benzyl and cyanomethyl resonance-stabilized radicals, 3-phenylpropionitrile is a likely component of the complex organics in Titan's atmosphere, motivating its structural characterization. Details of the modified line picking scheme, hyperfine constants and relative population ratios of the two conformers will be presented.

[1] A.O Hernandez-Castillo, Chamara Abeysekera, Brian M. Hays, Timothy S. Zwier, "Broadband Multi-Resonant Strong Field Coherence Breaking as a Tool for Single Isomer Microwave Spectroscopy." J. Chem. Phys. 145, 114203 (2016).