

## IMPROVEMENTS TO NEW PROGRAM FOR SPIN-TORSION-ROTATION & THE METHYL-PHENOXYL RADICALS

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A new program, written in Julia, has been written to simulate and fit spectra of radicals with 3-fold internal rotors. The program now uses a single diagonalization stage implementation of the Rho Axis Method to provide more direct usage of the wavefunction symmetries for the  $A$  states. The three different methyl positions provided test cases of potential spin-torsion coupling with varying internal barrier heights of about  $V_3 \approx 206 \text{ cm}^{-1}$  in ortho,  $V_3 \approx 64 \text{ cm}^{-1}$  in meta, and  $V_6 \approx 7 \text{ cm}^{-1}$  in para. Spectroscopic parameters determined from CCSD(T)/ANO0 calculations provided test cases for assigning states and simulating the spectra. The rotational spectra of ortho-, meta-, and para-methyl-phenoxy radicals was collected through Chirped-Pulse Fourier Transform Microwave Spectroscopy. The radicals were produced from the appropriate methyl anisole precursors through pyrolysis in a SiC pyrolysis source attached to a pulsed valve. The temperature of the reactor was monitored with an infrared camera and the production of the radicals was monitored with 118 nm photoionization -Time of Flight Mass Spectrometry. Once the optimal temperature of the pyrolysis source was determined, the rotational spectrum was recorded from 7.5 – 17.5 GHz. Each radical was fit as a closed-shell species using RAM36 and as an open-shell species using the new program which also included spin-torsion coupling terms.