UNTANGLING THE NEAR-IR HIGH RESOLUTION SPECTRUM OF THE METHYL PEROXY RADICAL

PATRICK DUPRÉ, PATRICK RUPPER, SHENGHAI WU and TERRY A. MILLER, *Department of Chemistry, Ohio State University, 120 W. 18th Ave, Columbus OH, 43210*.

The jet-cooled high resolution CRDS spectra of the methyl peroxy radical, CH_3OO and CD_3OO has been obtained for the weak $\tilde{A}\,^2A' \leftarrow \tilde{X}\,^2A''\ 0_0^0$ band. The rotational spectra of the isotopologue species exhibit very different structure. The hindered internal rotational involving methyl and O_2 groups is a source of this very different structure, due to the strong dependence of the tunneling splitting upon mass through the F parameter ($\sim 4.4\,\mathrm{cm}^{-1}$ for CD_3OO compared to $\sim 7.0\,\mathrm{cm}^{-1}$ for CH_3OO). We will discuss the formalism in the limit of the high torsional barrier in the light of the experimental results, emphasizing the spectral resemblances and differences.