Electronic excited state properties of organic hydroperoxides

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In this work the features of the electronic absorption spectrum of hydrogen peroxide, methyl peroxide and higher orger organic peroxides were explored. These molecules are important contributors to the OH radical budget in the atmosphere. Currently the rate of dissociation of high order organic peroxides (such as isoprene hydroperoxide) is modeled using the dissociation rate of methyl hydroperoxide which is not sufficient and is a source of errors in the predicted concentration of OH radicals. The purpose of this work is 1) to understand the spectral features of peroxides and 2) find the correct dissociation rates for organic peroxides that are present in the atmosphere.