UV SPECTRUM AND PHOTODECOMPOSITION OF PEROXYNITROUS ACID (HOONO)

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Peroxynitrous acid HOONO plays an important role in atmospheric chemistry. It is formed as a minor product by the chain-terminating reaction of NO_2 and OH, the main product being nitric acid, $HONO_2$. Peroxynitrous acid was first observed in an Argon matrix[1]. Its UV spectrum was recorded soon after[2]. In contrast to nitric acid, peroxynitrous acid is an unstable species and has not been seen in the gas phase at ambient pressure and temperature because of its short lifetime of a few seconds[3]. HOONO disintegrates readily through thermolysis and photodecomposition. These processes are not well understood and are investigated in the present work.

To this end, the UV spectrum was computed using both DFT and ab initio methods. Upon UV excitation, the molecule will break up to yield either HO_2 + NO or NO_2 + OH. The decay process was studied in detail by non-adiabatic dynamics on the lowest four electronic potential energy surfaces using the NEWTON-X package[4], interfaced with the MOLPRO and GAUSSIAN programs. From a statistical analysis of a large number of trajectories, we were able to obtain the fragment distributions for the two conformers cis-cis and trans-perp. Our analysis revealed that the cis-cis conformer produces 95% of HOO+NO and 2% of HO+ONO, whereas the trans-perp conformer yields HOO+NO with a 100% yield. The tropospheric photolysis rate constant was then obtained from the computed UV cross-section data and the actinic flux.

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