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Classical Trajectory Studies of the Hydrogen Peroxyl Radical HO_2 JAMIN PERRY, University of Missouri-Columbia, ALBERT WAGNER, Argonne National Laboratory, DONALD THOMPSON, University of Missouri-Columbia — The intramolecular dynamics, intramolecular vibrational redistribution of energy (IVR), isomerization and unimolecular dissociation of the hydrogen peroxyl radical, $HO_2^* \rightarrow H + O_2$ have been studied using classical trajectories. Mode specific effects are found to affect the IVR, isomerization and the rate of dissociation. Exchange of the hydrogen atom between the oxygen atoms increases the rate of energy transfer between the vibrational modes of the radical. The relaxation mechanism of the vibrationally excited radical embedded in a dense gas environment is also presented.

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