Public Abstract
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This dissertation is focused on studies of the classical dynamics hydrogen peroxyl radical (HO2), which is an important intermediate in combustion chemistry. The first study of this thesis is focuses on the dynamics of the isolated radical. Comparisons are made between the three potential energy surfaces (PESs) that have been used as models for the radical.The dynamics of isolated HO2 exhibit mutiple timescales that reflect properties of fast and slow energy transfer in the radical. The energy transfer is well represented by an analytic, coupled three-mode model.
The second study of this thesis is focused on the effects of pressure on the relaxation of the HO2 embedded in a dense gas environment. A method of simulating the radical in an argon bath is proposed and validated. The time-dependent decay of vibrational energy is found to be bi-exponential for all of the simulated pressures. Pressure dependent effects were found and comparisons to studies with similar findings and additional considerations for understanding this behavior are discussed.