

Abstract Submitted
for the PSF13 Meeting of
The American Physical Society

Rotational -Vibrational Energy Transfer in OH(v,J)+ Ar at High Pressures REZVAN CHITSAZI, DONALD THOMPSON, University of Missouri-Columbia — The exchange of energy in collisions of atoms, molecules and radicals has attracted interest since the introduction of kinetic theory and its subsequent applications in chemistry. We have studied the effects of pressure on the relaxation of excited OH radical. In most modeling of gas phase chemistry it is assumed that it occurs via isolated elementary bimolecular collisions; that is, the fundamental energy transfer and reactions occur between pairs of species. Our interest is to explore the relaxation of an internally excited radical at pressures for which the bimolecular collision assumption breaks down. We will present results for molecular dynamics simulations of the rotational-vibrational energy transfer for OH(v,J) in an Ar bath for internal energies up to the dissociation limit and over pressure and temperature ranges that include and exceed those achievable in the laboratory.

Thomas Sewell
University of Missouri-Columbia

Date submitted: 10 Oct 2013

Electronic form version 1.4