Abstract Submitted
for the DAMOP14 Meeting of
The American Physical Society

Studying inelastic collisions of H_2 and D_2 by means of ultrasonic experiments[1] JESUS PEREZ-RIOS, Physics Department, Purdue University, West Lafayette, IN 47907,USA, SALVADOR MONTERO, Laboratory of Molecular Fluid Dynamics, Instituto de Estructura de la Materia, CSIC Serrano 121, 28006 Madrid, Spain — An explicit formulation for the rotation-translation relaxation time in terms of state-to-state rate coefficients associated to inelastic collisions is presented. The formulation provides a tangible link between acoustic and gas dynamics, and quantum scattering calculations. The state-to-state rates needed for the detailed interpretation of relaxation of H_2 and D_2, including isotopic variant mixtures, have been calculated by solving the close-coupled Schrödinger equations. Relaxation related quantities (rotational cross section, bulk viscosity, relaxation time, and collision number) calculated from first principles agree reasonably well with acoustic absorption experimental data on H_2 and D_2 well below 293 K. This result confirms the proposed formulation, the quantum scattering calculations, and the potential energy surface employed.

[1]This work was partially supported by DOE, Office of Science

Jesus Perez-Rios
Physics Department, Purdue University, West Lafayette, IN 47907,USA

Date submitted: 31 Jan 2014 Electronic form version 1.4