Abstract Submitted
for the DAMOP17 Meeting of
The American Physical Society

Rate Constants for Fine-Structure Excitations in O - H Collisions with Error Bars Obtained by Machine Learning[1] DANIEL VIEIRA, ROMAN KREMS, University of British Columbia — Fine-structure transitions in collisions of $O(^3P_j)$ with atomic hydrogen are an important cooling mechanism in the interstellar medium; knowledge of the rate coefficients for these transitions has a wide range of astrophysical applications. The accuracy of the theoretical calculation is limited by inaccuracy in the ab initio interaction potentials used in the coupled-channel quantum scattering calculations from which the rate coefficients can be obtained. In this work we use the latest ab initio results for the $O(^3P_j)$ + H interaction potentials to improve on previous calculations of the rate coefficients. We further present a machine-learning technique based on Gaussian Process regression to determine the sensitivity of the rate coefficients to variations of the underlying adiabatic interaction potentials. To account for the inaccuracy inherent in the ab initio calculations we compute error bars for the rate coefficients corresponding to 20 % variation in each of the interaction potentials. We obtain these error bars by fitting a Gaussian Process model to a data set of potential curves and rate constants. We use the fitted model to do sensitivity analysis, determining the relative importance of individual adiabatic potential curves to a given fine-structure transition.

[1]NSERC

Daniel Vieira
University of British Columbia

Date submitted: 29 Jan 2017 Electronic form version 1.4