

Interpolated Potential Energy Surfaces for Theoretical Studies on the Dynamics of Interstellar Reactions

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Abstract. Systematic construction of molecular potential energy surfaces is performed by interpolation on sparse sets of ab initio data points, following a methodology developed in recent years. The potential energy surfaces thus constructed have been used in theoretical studies of the molecular dynamics of some interstellar reactions. Theoretical values of the rate coefficients for the reactions (which can be based on classical or quantum dynamics simulations) are among the most important outcomes this work provides for interstellar chemistry models. The accuracy of these predicted rates depends upon factors such as numerical error of the interpolation, quantum chemistry approximations employed to calculate the data points, and the approximations in the dynamics simulations.

We have applied this methodology to some molecular systems involved in deuterium fractionation processes in the interstellar medium. We have constructed several potential energy surfaces converged to chemical accuracy for molecular dynamics, and calculated rate coefficients based on classical dynamics for conditions similar to those of the interstellar medium.

Keywords. ISM: kinematics and dynamics, molecular processes
