INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Thesis Title: **Scattering Studies of Proton Transfer Reactions between Rare Gas Atoms**

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SHORT ABSTRACT

Interactions between proton and light rare gases often occur in interstellar spaces and planetary atmospheres, which play important role in astrochemistry. In this thesis, global analytical potential energy surfaces are generated on the ground electronic states using high level ab initio (CCSD(T)/aug-cc-pVQZ) energies for two triatomic proton bound rare gas systems, [HeHNe] + and $[NeHNe]^+$. Linear geometries with the hydrogen in between the rare gas atoms are found to be the most stable structures for both the systems. Bound states and eigen energy spectrum are calculated for zero total angular momentum for those most stable structures. Reactive scattering dynamics are performed for the proton transfer reactions, He + $NeH^+ \rightarrow HeH^+$ + Ne and the reverse process and Ne + $NeH^+ \rightarrow NeH^+$ + Ne by using time-dependent quantum mechanical, time-independent quantum mechanical and quasiclassical trajectory calculation methods on the analytical potential energy surfaces. State averaged reaction attributes, i.e., reaction probabilities, integral cross sections, rate constants are calculated for these reactions for different initial ro-vibrational states. State-to-state dynamics as well as mechanistic paths at different collision energies have also been investigated for these reactions starting from ground reactant ro-vibrational states. Fortran programs are written to compute the eigen states of the stable complexes and to investigate the adiabatic reaction dynamics by following time dependent wave packet propagation method. Shared memory and message passing interface parallelization algorithms are implemented in the codes. Fortran programs are also written to calculate quasi-classical trajectories for a triatomic bimolecular reaction and to analyze those trajectories.