Synopsis

The studies on the atomic and molecular collision processes are essential for understanding the intermolecular forces and also the mechanisms involved in such processes. The collision processes may broadly be divided into two classes, viz., elastic and inelastic.

The elastic scattering studies have till now been mostly used for the study of intermolecular forces as experimental inelastic scattering data are as yet very scanty and not sufficiently accurate. The theories for inelastic processes are also not sufficiently developed to allow direct determination of intermolecular forces.

For the diatomic and polyatomic gases, the most important inelastic process in the thermal energy range is the rotational excitations by collision with a structureless particle or another molecule. Apart from fundamental interest, these studies have become very much relevant to space physics as they determine the cooling rates and also the properties of the interstellar medium.

In this thesis certain aspects of the elastic processes, viz., inversion from the total scattering cross sections and rainbow structure have been dealt with. On the inelastic side work has mainly been concentrated on the purely rotational excitations of molecules and molecular ions in collision with electrons, positrons and hydrogen molecule. The vibrational-rotational excitations of the simplest hetero-nuclear and heteropolar molecular ion (HeH)+ have also been studied.
The contents of the thesis have been divided into two parts, I and II. Part I deals with the studies on elastic processes and Part II with those on the inelastic processes. Each part consists of four chapters, the details of which are given below.

Part I

The Chapter I contains an Introduction to the elastic scattering processes which have been dealt in the thesis.

The Chapter II presents a Review of the theoretical work done on the elastic scattering processes with emphasis on the rainbow and glory scattering phenomena and inversion methods.

The Chapter III describes the theories for elastic scattering, classical, quantal and semi-classical. The semi-classical theory for rainbow and glory scattering has been given in detail. The Firsov's method for inversion has also been described.

The Chapter IV consists of two sections. In Section I, the method of inversion from the energy dependence of total cross sections has been critically analysed for the He-He system. Due to the lack of experimental data over the whole energy range required for inversion, some data had to be generated theoretically. The results show that this method of inversion is capable of yielding reliable informations on the intermolecular potential. In Section II, the positions of a large number of maxima and minima have been calculated for the Kihara core potential by using the
uniform approximation. The results for the Lennard-Jones (12:6) potential have also been obtained as a special case for the Kihara potential. The experimentally obtained rainbow structure has been analysed for several systems by using the results obtained by us to yield informations about intermolecular forces and some interesting conclusions have been drawn.

Part II

The Chapter I contains an Introduction to the rotational excitation processes which have been studied in the thesis.

The Chapter II gives a brief Review of the theoretical work done on the rotational and vibrational-rotational excitations of molecule and molecular ion in collision with a structureless particle or another molecule.

The Chapter III deals with the theories for rotational excitations of molecules. Both the time independent and the time dependent methods have been described. For the time independent method starting from the close coupling method of Arthurs and Dalgarno, other approximations have been obtained. For the time dependent methods, starting from the general expression the various approximation methods have been described.

The Chapter IV contains four sections, the details of which are given below.
In Section I, the rotational excitations of CO and NO by slow electron impact has been treated by using the Born approximation. The special feature of this study is the inclusion of the short-range interaction in the interaction potentials. It has been shown that even for slow electron collisions the short-range interaction plays a significant role for the molecules under consideration.

In Section II, the vibrational - rotational excitations of (HeH)+ molecular ion have been treated by using the first order time-dependent perturbation theory. The energy range has been chosen so that the trajectories are non-penetrating. The results show the very significant influence of the dipole term in the interaction potential on the vibrational-rotational excitations of molecular ion having permanent dipole moment.

In Section III, the purely rotational excitations of HD+ ion in collision with an electron or positron has been treated by a semi-classical time-dependent perturbation theory. For electron-HD+ collisions, the effect of penetration of the charge cloud has been considered. The results have brought out some very interesting features of rotational excitations of molecular ions.

In Section IV, the rotational excitations of the linear polyatomic molecule HCN in collision with H2 molecule has been treated by the exponential approximation. H2 has been taken to be in the states \( j=0 \) and \( j=1,2 \). In the latter cases the electrostatic interactions influence the rotational excitation process.