PREFACE

One of the most interesting developments in Astrophysics during the last decade has been the discovery of a large number of molecules in interstellar clouds which has revolutionized our knowledge about these objects. In addition to those for neutral molecules, line emissions for molecular ions have also been observed with the help of radioastronomical techniques. Attempts are being made to obtain information about these clouds from the line emission data. For this purpose different models for clouds have been constructed, such as the gravitational collapse and the turbulent models. In the collapse model, the starting point is the radiative transfer model of Sobolev (1960) as developed further by Castor (1970) and Lucy (1971). In this model, due to the presence of a large velocity gradient, a photon emitted at a certain point in the cloud either is absorbed in the immediate surroundings or escapes so that the transfer of radiation depends only on the local physical conditions such as number density and kinetic temperature. The population amongst different rotational levels of the molecule are determined by the radiative transitions due to the cosmic ultraviolet radiation and collision induced rotational excitation of molecules. In addition, a process which is known as radiative trapping (Scoville and Solomon 1974) also occurs in optically thick clouds. From a study of the line intensities together with its variation with the distance from the centre of the cloud it is possible to determine the physical conditions existent...
in the cloud. For simplicity the cloud is assumed to be spherical in shape with large scale velocity gradient due to collapse and also a density gradient is assumed. Some general calculation of brightness temperatures of the spectral lines of a number of molecules using this model was first made by Goldreich and Kwan (1974). Gerola and Sofia (1975) were the first to apply this model for the interpretation of the spectral data of CO and HCN obtained from Orion A cloud. de Jong et al (1975) also made extensive general calculations using this model.

Although Gerola and Sofia (1975) could explain the line intensities fairly well in terms of their model and also obtained values for the physical parameters such as density, temperature etc. in the cloud there were several anomalies which could not be explained. However, these works have shown the potentials of using the spectral data in determining the physical conditions in the cloud.

Another model of the cloud which has been suggested is the turbulent model. In this model the cloud is assumed to be supported by supersonic turbulence. Arguments in favour of the turbulent model has been put forward by a number of workers (e.g. Zuckerman and Evans 1974). However, there are a number of serious difficulties with this model. One of them is that to maintain the turbulence against decay the existence of a strong source of mechanical energy is required. As the decay time must be comparable to the time it takes a strong shock to propagate across the largest eddies, the requirement for
the maintenance of turbulence is quite serious. The turbulence hypothesis also fares poorly in accounting for the fact that the emission lines observed from different isotopes of the same molecular species have often similar shapes with different intensities.

On the other hand, the gravitational collapse model with the consequent large scale velocity gradient has no such difficulty as mentioned above and seems to be on balance a better representative of the actual conditions in the interstellar clouds. However, more recently it has been suggested by Kwan (1978) that the turbulence holds very near the centre of the cloud and on the outer side the spherical collapse model holds, though this model is not likely to be universally applicable (Phillips et al 1979).

Thus, it is seen that till now only preliminary work on the interpretation of the spectral data obtained from interstellar clouds has been done and a lot of work remains to be done. In this thesis attempt has been made to obtain some information about the physical conditions existent in interstellar molecular clouds and particularly in Orion A cloud by using the collapse model.

As stated earlier, the population distribution amongst the different rotational levels of a molecule which determines the line intensities is dependent on the rate coefficients for rotational excitation by collision. It may be mentioned that at temperatures existent in interstellar molecular clouds only rotational excitation
process is important. In such clouds, the most abundant molecular species is H$_2$. The calculations of line intensities have been done mostly by considering the rate coefficient for rotational excitation of the molecule by collision with H$_2$. However, the existence of electrons in such clouds is a certainty, although their concentration is uncertain. The estimates of the relative concentration of electrons to that of H$_2$ vary from $10^{-4}$ to $10^{-8}$. For molecular clouds having infrared sources such as Orion A, the concentration of electrons is likely to be high. For strongly polar molecules such as CS, HCN etc. the rate coefficients for electron–molecule collisions are expected to be much higher than the corresponding values for H$_2$–molecule collisions so that these are likely to affect line intensities of these species although the electron concentration is much lower than H$_2$ concentration.

If the densities of the colliding molecular species in the interstellar cloud are not sufficiently high there is departure from the local thermodynamic equilibrium (L.T.E.). Under non-L.T.E. conditions the line intensities are sensitively dependent on the rate coefficients. Thus for a proper interpretation of the line intensities it is necessary to know the rate coefficients for rotational excitation. For collision with H$_2$, rate coefficients under interstellar conditions have been calculated for a number of systems such as H$_2$–CO, H$_2$–HCN, H$_2$–N$_2$H$^+$ etc. by using the close coupling method. For electron–molecule collision such calculations have not been done extensively. Dickinson and Richards (1975)
by using the unitarized time dependent perturbation theory have obtained a comparatively simple formula for the rate coefficient for electron–molecule collisions which is expected to hold well for molecules with low dipole moments. For strongly polar molecules and molecular ions the rate coefficients for rotational excitation by electron impact which are valid under interstellar conditions are not available. Attempt has been made in this thesis to obtain these information.

The thesis consists of two parts. In Part I, the calculation of rotational excitation cross section and rate coefficients for electron–molecule and electron–molecular ion collisions has been dealt with. In Part II attempt has been made to interpret the spectral data for CO and HCN as obtained for Orion A cloud using the spherical collapse model and to obtain information about the physical conditions existent in that cloud. The effect of electron–molecule collisions on the brightness temperatures of the spectral lines for optically thick clouds has been assessed and method for the determination of hydrogen and electron densities in interstellar clouds has been suggested. The actual contents of the thesis have been given below in some detail.

Part I

Rotational Excitation of Molecules and Molecular Ions by Electron Impact.

In Chapter I, the work done till now on the calculation of rotational excitation cross section of electron–molecule and molecular ion collisions has been reviewed.
In Chapter II, the different methods used for the calculation of electron–molecule rotational excitation cross section under interstellar conditions have been described.

In Chapter III, the rotational excitation cross sections and rate coefficients for e–CO and e–HCN collisions under interstellar conditions have been obtained by using the Gordon's technique for the close coupling method. The cross sections and rate coefficients thus obtained have been compared with the Born and unitarised time dependent perturbation calculations.

In Chapter IV, a generalised expression for the rate coefficient for rotational excitation of molecular ions by electron impact under interstellar conditions has been obtained from the first order perturbation theory. The expression has been obtained by considering only the electron–dipole term of the interaction potential which is also the most dominant term. The effects of short–range and electron–quadrupole interactions have been assessed. The importance of electron–ion collisions compared to that of H₂–ion collisions for the interpretation of the spectral data obtained for ions from interstellar sources has been estimated.

Part II

Interpretation of Rotational Spectra Observed from Molecular Clouds.

In Chapter I a brief introduction has been given on the physics of interstellar clouds. Observations of spectral lines of some
important molecules have been described. The work done till now on the interpretation of these data together with the cloud models used have been reviewed.

Chapter II has been divided into two sections. In Section A the spherical collapse model has been used together with the simultaneous existence of the density and velocity gradients to interpret the rotational lines for $^{12}\text{CO}$ (2−1 and 1−0) obtained from Orion A cloud. The brightness temperature $T_B$ as a function of the radial distance from the centre of the cloud have been considered. In order to explain the data it has been assumed that the density at least in the central part of the cloud varies as $1/r$ where $r$ is the distance from the centre. In the earlier calculation done by Gerola and Sofia (1975) the density of $\text{H}_2$ was taken to vary as $1/r^2$ which could not explain some of the features observed for the 2−1, 1−0 lines of CO. In Section B with the data for the 1−0 line of HCN we have attempted to check the density variation of $\text{H}_2$ in the central part of Orion A cloud as obtained from the 2−1, 1−0 lines of $^{12}\text{CO}$. The results obtained for 1−0 line of HCN together with the sample calculations done for $^{13}\text{CO}$ show that at least near the centre of Orion A cloud $1/r$ dependence of the density of $\text{H}_2$ is a better representation of the actual state of affairs than the $1/r^2$ dependence assumed earlier by Gerola and Sofia (1975). However, best results for the 1−0 line of HCN have been obtained by assuming an exponential variation of the density of HCN with $r$. 
Chapter III has also been divided into two sections. In Section A the effects of electron-molecule collisions on the intensities of rotational spectra of polar molecules have been estimated for a range of conditions existent in interstellar clouds by using the radiative transfer model with a large velocity gradient. The spectral lines for the strongly polar molecules HCN and CS have been investigated and for comparison the weakly polar molecule $^{13}$CO has also been considered. For HCN and CS the effect of electron-molecule collision on the brightness temperature has been found to be quite significant at electron concentrations which may be present in the clouds with infrared sources like Orion A. From the results obtained for the lines of $^{13}$CO, it has been suggested that these data may be used for the determination of $H_2$ density throughout the cloud. Since $^{12}$CO lines are thermalized near the centre of the cloud, these data may be used for the determination of kinetic temperature of the cloud. The data for the strongly polar molecules like HCN, CS etc. may thus be fitted to yield an estimate of electron concentration in the cloud. By utilising the method suggested above in Section B the molecular hydrogen densities in six interstellar molecular clouds have been determined from the spectral data for $^{12}$CO and $^{13}$CO. The results indicate that in the central part of each cloud the density of $H_2$ decreases exponentially with the distance from the centre. The electron density near the centre of Orion A cloud has been determined from the spectral data for HCN. For the other clouds considered, the electron densities appear to be too low to affect the spectral intensity.