CHAPTER 1
INTRODUCTION

1.1 GENERAL

Molecular spectroscopy is a fundamental tool used in various research areas such as astrophysics, chemical physics, geophysics, combustion physics, environmental science and so on. Especially, it has played a major role in the research on astrophysical sources containing molecular species (Herzberg 1950). Detailed analysis of the spectral energy/intensity distribution in astrophysical sources makes it possible to determine the various physical conditions such as the relative abundances, temperature, pressure, strength of the magnetic fields and proper motion of the medium, etc.

The quantitative distribution of the molecular abundances in the universe is a classical problem in astronomy, astrophysics and cosmo-chemistry (Dalgarno and Layzer 1987). The reasons, why the astrophysicists are interested in determining the abundances of the atomic and molecular elements, are:

(1) To know the primordial composition of the solar system and its relation to the present composition of the earth and other planets. Such data might throw some light on vexing problems connected with the origin and chemical history of the earth (Anders and Grevesse 1989).

(2) A knowledge of the composition of the local part of our galaxy is needed for the construction of models of the Sun and stars, and for a complete understanding of physical and chemical processes taking place in the stellar atmospheres and the interstellar medium (ISM).

(3) The predicted/observed abundance distribution of atomic or molecular elements enables an astrophysicist to test the hypotheses that have been proposed for element formation.
Various astrophysicists have therefore independently taken up systematic programmes of investigations of selected diatomic molecular spectra. The results of the analysis on the experimental/theoretical study of the molecular abundances in above mentioned astrophysics and other fields are so important. Hence, it is necessary to have systematic investigation of the spectra of the molecules which are either found to be present or suspected to be present in different astronomical sources.

Especially, in the study of atomic and molecular abundances, the astrophysicists do the spectroscopic research in two ways: (1) wavelength studies, from which atomic and molecular structure constants may be derived from the inferred energy level separations and (2) intensity studies, from which the transition probability data and physico-chemical conditions in the observed light source may be inferred. Both of these ways of research find many applications in astronomy and astrophysics.

The significance of knowledge concerning diatomic molecules in the solar and stellar spectra has been stressed by astrophysicists (Herzberg 1950). Many diatomic molecular species are present in various astrophysical sources. The laboratory investigations have also reached a stage of advancement especially for atomic and diatomic molecular species. However, the theoretical studies on such astrophysically significant atomic and molecular species for the estimation of atomic/molecular abundances in the astrophysical sources are not enough. Also, quantitative theoretical analysis of the spectra of the astronomical sources and of the processes that populate the atomic and molecular energy levels that give rise to emission and absorption by these sources, require accurate data on the transition frequencies/wavelengths, transition probability parameters, dissociation energies, ionization potentials, etc.
1.2 SIGNIFICANCE OF THE PROBLEM

The spectroscopic studies on the radiation received from an astrophysical source give the information about mass, size, pressure, temperature, magnetic field and the proper motion of the extra-terrestrial bodies as well as the intervening space. Such important studies are mainly governed by the theoretical studies and experimental studies on the astrophysically significant atoms or diatomic molecules. The theoretical studies refer to the calculation of some molecular parameters by using some empirical relations and the experimental studies mean that the observation of the spectrum of atoms/molecules both in laboratory and from astrophysical objects.

For the estimation of above mentioned physico-chemical parameters, it is necessary to have a theoretical background or knowledge on the corresponding transition probabilities like Franck-Condon (FC) factors, r-centroids and potential energy curves for the respective bands in a band system of a molecule. Reliable values of FC factors and r-centroids are essential to arrive at the variation of electronic transition moment, band strength and vibrational temperature of the source (Rajamanickam 1985 & 1987). The FC factors play an important role in determining the rate constant of non-radiative decay (Straughan and Walker 1976).

As widely known, the FC factors are not only useful for the calculation of individual values, and their band-by-band application, but are also useful in studies of astrophysical atmospheres which contain molecular species. In the case of molecules, which are expected to be present in the astrophysical sources, the transition probabilities give an indication of the most probable transition likely to be seen in the spectra of celestial objects if the transition probability is high. As pointed out by Frisch (1971), a knowledge of the electronic oscillator strength and FC factors is necessary to convert the absorption/emission data into molecular optical depths and column densities; in particular, she noted the strong dependence of these
quantities on the ratio of FC factors $q_{(0,0)}/q_{(1,0)}$. Also, the accurate knowledge of the FC factors of diatomic molecules is of fundamental importance for diagnosis of physical conditions existing in astronomical and aeronomical light sources, for studies of molecular structure and for chemical studies involving reactions between atoms and molecules (Ramjee et al 1982).

The concept of r-centroids has been much used since then in the interpretation of intensity measurements on many band systems of importance in astrophysics, atmospheric physics, space physics and chemical physics to determine the variation of electronic transition moment with internuclear separation, and thereby to derive band strengths, and other molecular transition probability parameters (Nicholls et al 2001). The smooth relationship between r-centroids and wavelengths should provide a useful bridge between experimental measurements, which are often expressed as a function of wavelengths and theoretical studies, which are often made in terms of internuclear separation (Miroslav Kuzmanovic et al 2005).

Therefore, a number of workers have undertaken theoretical studies to provide FC factors, r-centroids and potential energy curves, etc., of the diatomic molecules which are of importance in astrophysics, gas kinetics, molecular spectroscopy and combustion processes (Singh 1988).

As already mentioned, by using the FC factors and r-centroids, the band strengths, relative band strengths and the vibrational temperature of the source could be calculated. From the obtained temperatures, the stars can be arranged in a temperature sequence (Merril et al 1962; Straughan and Walker 1976; Pavlenko 1999). The presence of molecules is seen in the late type stars called M- and S-type stars, since the surface temperatures of such stars are below 4000 K. In the case of Sun which is a G-type star, the atomic and molecular species are dominant, since the surface temperature is about 5800 K and the temperatures in the layers of sunspots
are even below 5800 K. Hence, the solar spectrum contains the signatures of many diatomic molecules due to the fact of the existence of such lower temperatures.

In the sunspots, the high magnetic field strength blocks a part of the radiation from star interior and hence, there exists a significantly reduced temperature in the sunspot umbra. These relatively cooler regions therefore allow the existence of various diatomic molecular species. The study on the identification of molecules in that atmosphere will be useful for an understanding of the physico-chemical conditions in sunspots and of their changes which is mainly dependent on the solar activity.

The sunspot umbral spectrum at high resolution comprises of a large number of rotational lines of various diatomic molecules like \( C_2 \), CN, CH, CaH, FeH, MgH and TiO, etc. Many of these molecular lines have been used in the observations of the evershed flow in sunspot penumbrae (Kulaczewski et al 1990; Uitenbroek et al 1994), for the estimation of excitation temperature at the layer of formation in umbrae and for evaluating the isotopic abundances, as in Wallace et al (1999).

In view of these applications, in the present study, the emphasis is laid on the study of molecular spectra of the diatomic species present in the solar atmosphere, especially in the umbrae of sunspots. Actual theoretical investigation of some of the diatomic molecules, likely to be present in sunspots, are first carried out followed by a search to identify the presence of the molecular species in high resolution and high quality spectra of sunspot umbrae.
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