STUDY OF THE SPECTRA OF SOME DIATOMIC MOLECULES (BiF, PbF and PbCl)

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SUMMARY

The thesis embodies a detailed and systematic analysis of the emission spectra of the diatomic molecules BiF, PbF and PbCl. A high frequency discharge tube source was found to be the best source to excite these molecules. For recording the spectra, a two metre plane grating spectrograph has been used. For the purpose of vibrational analysis, the spectra have been photographed in the lower orders of the grating. The rotational structure of individual bands could be resolved in higher orders of the grating only. The analysis of the band systems were carried out using conventional techniques.

The thesis is divided into two parts. Part 1 includes an introduction to the subjects, a historical survey of the work done so far on the molecules under the present study and a few other molecules which are spectroscopically similiar to

them. Inorder to make the thesis self-contained a brief account of the vibrational structure of bands and intensity distribution in a band system, rotational structure of a simple band system are also included in the introduction which forms the first chapter. Second chapter deals with the historical survey and the main object in selecting the molecules is elucidated. The sources which are generally employed in the study of the spectra of diatomic molecules in emission are discussed in the third chapter. The high frequency discharge tube source is described in detail as it served to excite the spectra of molecules reported in the thesis.

Vibrational and rotational analyses of different band systems and results obtained therefrom are included in part II. Electron configurations of various electronic states of molecules under consideration and conclusions drawn from the

present study are also included in Part II.

Chapter four deals with vibrational and rotational analyses of C - X system of BiF molecule. Correctness of the vibrational assignments reported by earlier workers have been checked by a reanalysis of vibrational spectrum. Rotational analyses of 0,0 and 0,1 bands of $C_1 - X_2$ and $C_2 - X_3$ systems of BiF molecule have been carried out. Observed Λ - doubling for the upper state of $C_1 - X_2$ system of BiF molecule has been discussed in detail.

In chapter five, spectrum of PbF molecule has been discussed. Vibrational assignments given by previous workers have been checked by a reanalysis of vibrational spectrum. $A - X_1$, $B - X_1$ and $B - X_2$ systems of PbF molecule have been studied in detail. Double headed nature of bands in the $A - X_1$ system has been confirmed

from the analysis. Spin - splitting and Λ - doubling observed in the spectrum of PbF molecule are dealt with in detail.

Chapter six deals with vibrational and rotational analysis of $A - X_1$ system of PbCl molecule. Reanalysis of vibrational spectrum of $A - X_1$ system of PbCl molecule has been carried out inorder to check the vibrational assignments given by earlier workers. Rotational analyses of 1,1 and 2,1 bands are carried out and the results obtained are also discussed.

In the last chapter, electronic configurations of BiF, PbF and PbCl molecules have been discussed in detail. Observed phenomena like spin - splitting, Λ - doubling etc of spectrum of molecules under consideration have been correlated with the theory of electronic structure. Similarities observed in the spectra of PbF and PbCl molecules have been discussed in the light of

electron configurations. Spectrum of BiF molecule in the ultraviolet region ($C_1 - X_2$ and $C_2 - X_3$ systems) has close similarities with the analogous molecule SbF. Conclusions regarding nature of energy levels drawn from the present study help to correlate nature of energy levels of BiF and SbF molecule.

C O N T E N T S

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