SUMMARY


Chapter 1 deals with the historical review and importance of the AlO molecule and also the statement of the problem. In this chapter it is stated that the AlO molecule has astrophysical significance and therefore the spectroscopic studies of this molecule are being pursued actively from last 60 years. With the improved high resolving power instruments the spectra of AlO were recorded and analyzed by various workers. The seven electronic states are known to this date. 10 electronic transitions between the different states are known. Out of them the B-X and C-X transitions are extensively studied. The deperturbation analysis of the bands in the D $^2\Sigma$ - A $^2\Pi$, transitions are relatively less studied. This motivated us to undertake these studies. Moreover the FC factors of A-X, D-X, D-A, D-B etc systems are reported for the first time. The Reduced Potential energy Curves (RPCs) of several isoelectronic molecules to AlO have been done for the first time.
The second chapter is related to the Fourier Transform Spectrometer (FTS) and excitation of AlO. Several researchers used different methods for the excitation of AlO, but in present case the microwave discharge was found suitable to record the bands of AlO. Small amount of aluminum trichloride was heated in a quartz boat in presence of oxygen and argon gas. Argon flow at 10 Torr was helpful in getting the good spectrum. A power of 2450 MHz at 150 Watt was applied to a discharge tube gave a proper spectrum. Several advantages of FT spectrometer are discussed in this chapter.

In Chapter 3, the deperturbation analysis is reported. The rotational analysis of seven bands of D-A system could help to get the accurate constants for A $^2\Pi_i$ state. Using these constant and fixing them with the constants of other states the perturbations were calculated with the help of PGHOPHER program. Perturbation constants were thus calculated.

Chapter 4 deals with the Franck-Condon factors and r-centriods of A-X, D-X, D-A and D-B system. These FC factors obey the Franck-Condon principle.
Chapter 5 is the last chapter which contains the studies of potential energy curves, RKR curves and Reduced Potential energy Curves. The quest of suitable empirical potential curve is still on. We have examined the well established Hulbert – Hirschfelder (H-H) potential, extended-Rydberg potential and Zavistas potential functions for the X \( ^2\Sigma^+ \) state of AlO molecule. We observed that the percentage deviation is the minimum for the extended – Rydberg potential function as compared to H-H and Zavistas’ potentials.

The Reduced potential energy curves (RPCs) of six isotopic molecules to AlO, namely CaH, BeCl, BS, CP, SiN and MgF are studied for their ground states. The RPCs show a perfect similarity with their respective RKR curves. This is one of the properties of the RPC. All the RPC’s also obey other rules of RPC’s. For example they have a minima at (1, 1) coordinate. In the combined RPC’s it is seen that they never intersect each other. It was also noticed that the reduced masses of BS and CP are very close to each other resulting in a very close, almost overlapping RPC’s of each other. It is also observed that the RPC of the lightest molecule CaH having \( \mu \) as 0.9832 lies innermost whereas the RPC of the heaviest molecule MgF having \( \mu \) as
10.6047 lie outermost. All other molecule shows orderly behavior in their RPC’s.

Finally the bibliography of classical and updated references is given.