CHAPTER V
CONCLUSION

Some of the major achievements of this project are summarized below:

1. We have successfully completed the project and raised the profile of UV spectroscopy to a new height. Other dimensions have been added.

2. Our first and foremost objective was to add authenticity to the methodology to apply derivatisation technique to analyses intricacies involved in a simple looking UV spectra. We are pleased to say that we have succeeded in our efforts beyond our expectations.

3. We have established that derivatisation technique is far more powerful and reliable than it was thought to be.

4. We have observed that this technique is so sensitive that it can identify species even in such a trace amounts where other analytical techniques fail (for e.g. HPLC).

5. The analytical power of this technique is so versatile that it can unearth such informations which require very sophisticated instruments e.g., Circular Dichroism spectrometer. Through this technique one can unearth even such information which even CD spectrometer can’t provide e.g., when we recorded CD spectra of our target molecule in polar and hydroxylic solvents in the π→π* region, featureless spectra without any vibrational transitions were observed while through our technique we observed beautiful spectra with all the expected features.

6. By applying this technique one can identify with fair amount of accuracy intermediates formed during the chemical reactions. Such information is of great use for the chemist to interpret the reaction mechanism. To the best of our knowledge very few techniques e.g., ESR spectroscopy etc. are able to provide this information.

7. We have successfully isolated and identified the vibrational transitions buried under intense bands in the π→π* region where usually the conc. of the solutions is very
very low of the order of $10^{-5}$ M. To the best of our knowledge no instrumental technique in the world of analytical chemistry exists which can perform such job with ease and accuracy.

8. Eastwood et al carried out an extensive theoretical study of acetone in a gas phase model and postulated that its electronic band in $n \rightarrow \pi^*$ region must show vibrational transitions at 262 nm, 270 nm, and at 278 nm. We have reported (from our lab) with remarkable accuracy the presence of these bands in solution phase just in simple derivative spectra. In fact this information was the first accurate information which we used as a reference line in other interpretations. To the best of our knowledge the isolation and identification of vibrational signals in such a simple manner that too in a solution phase spectra are being reported for the first time. No one has succeeded so far. In fact we have paved the way to determine vibrational transitions in a UV band just by carrying out a simple derivatisation of electronic band. This is our most worthy contribution because according to Born Oppenheimer rule “The electronic transitions are always accompanied by vibrational transitions”. In gas phase spectra these kinds of transitions have been reported but very rarely in solution phase.

**Studies with Cyclohexenone**

Up to this stage we have understood how to extract best possible results from simple UV spectra. We proceeded to apply it on cyclohexenone. This study was vital, because our target molecule testosterone is actually a substituted cyclohexenone. Therefore this molecule and testosterone should have some commonality, hence spectral study with this molecule will provide foundation.

The conclusions of the studies with this molecule are summarized below:

1. UV spectra of this compound in different solvents are reported in zero derivative modes. The bands positions and solvent effect have been discussed accordingly. We have extracted better and more accurate results through our approach.
2. We were able to mark very clearly the vibrational bands associated with both \( \pi \rightarrow \pi^* \) and \( n \rightarrow \pi^* \) transitions. **To the best of our knowledge this is being reported for the first time.**

3. Conformational analysis of this molecule has been done through Circular Dichroism (CD). The explanations have been provided through extrapolation of CD curves. We obtained the same observations rather in a clear cut manner through simple 1st derivative spectra. Bands due to different conformers were isolated and precisely marked through higher derivative spectra. We feel that 1st derivative spectra can complement CD spectroscopy and some time can provide better results.

**Studies with Testosterone**

Our target molecule is basically a substituted four membered cyclohexenone. Therefore, this molecule should show some of the transitions observed with cyclohexenone with some red shift due to substitution and may be some additional features. This molecule has 8 asymmetric carbon atoms and should be in equilibrium with 64 epimers. But, in natural steroids the rings; B/C and C/D are always transfused and this in turn reduces the number of stereoisomers with few exceptions. Its spectra in the zero derivative mode with simple transitions are reported.

1. We recorded the spectra in different solvents and through derivatisation isolated and marked electronic bands with its associated vibrational transitions in both \( \pi \rightarrow \pi^* \) and \( n \rightarrow \pi^* \) regions.

2. We succeeded in identifying some of the spectral features as due to the twist in the rings, which have been studied by employing elaborate techniques.

In the end we would like to sum up briefly our unique contribution through this project. These are:

1. Derivative Spectroscopy is far more powerful, sensitive and accurate then it had been realized.

2. Through this technique one can unearth and unravel so many spectral features which are possible only through sophisticated and elaborate techniques.
3. We have very successfully demonstrated and isolated vibrational transitions as part of electronic excitation. We wish to clarify that our conclusions are based only on our study with keto group molecules.

**Future Scope of this Project**

As mentioned above derivative spectroscopy has tremendous potential, which need to be fully realized by studying few more systems, particularly with those molecules which do not have keto group as part of the structure. It needs to be applied on such phenomenon where molecule is in equilibrium with its own other forms and the energy differences are very small.