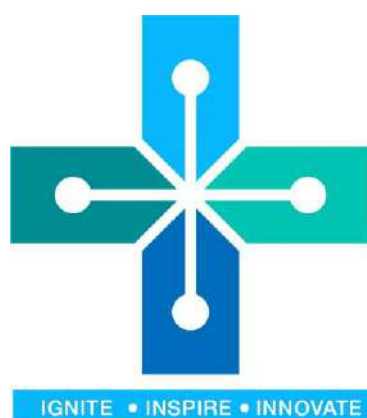


GUIDELINES FOR THE PREPARATION OF SYNOPSIS AND Ph.D. THESIS



Research and Development Wing

St. Peter's Institute of Higher Education and Research

(Deemed to be University U/S 3 of the UGC Act, 1956)

AVADI, Chennai 600 054

2023



Dr. S. Gunasekaran, M.Sc., Ph.D., D.Sc.

TANSA Awardee

Dean, Research & Development

St. Peter's Institute of Higher Education and Research

(Deemed to be University U/S 3 of the UGC Act, 1956)

AVADI, Chennai – 600 054, Tamil Nadu, India.

E-mail: deanresearch@spiher.ac.in

13-03-2023

Dear Scholars and Supervisors,

It is with great pleasure that the guidelines for the preparation of synopsis and thesis for the Doctor of Philosophy (Ph.D.) program in our esteemed institution are introduced. The Dean of Research and Development has had the privilege of overseeing the development of these guidelines, aimed at providing clear instructions and standards to ensure the highest quality of scholarly work and research output.

The preparation of a synopsis and thesis represents a significant milestone in the Ph.D. journey, symbolizing years of rigorous research, critical analysis, and scholarly exploration. These guidelines have been designed to assist scholars and supervisors in effectively navigating the process and producing research that meets the highest standards of academic excellence.

The guidelines cover various important aspects related to the preparation of both the synopsis and the thesis, including structure, formatting, citation styles, and overall organization. Scholars and supervisors will find detailed instructions on crafting a clear and coherent research synopsis and thesis that effectively communicate research objectives, methodology, findings, and conclusions.

Appreciation is expressed to the members of the research advisory council involved in the development of these guidelines. Their expertise and commitment to excellence have been invaluable in shaping this comprehensive framework.

Scholars are congratulated on reaching this crucial stage of their Ph.D. journey, with encouragement to familiarize themselves with these guidelines and use them as a valuable resource throughout the preparation of their synopsis and thesis. Their dedication, rigorous research, and scholarly contributions will undoubtedly contribute to the advancement of knowledge in their respective fields.

Gratitude is extended to the supervisors for their mentorship and guidance to the scholars. It is believed that these guidelines will serve as a valuable tool in facilitating effective supervision and providing constructive feedback to help scholars produce high-quality research.

Wishing all scholars success as they embark on the preparation of their synopses and theses, with hopes that this experience will be fulfilling and transformative, propelling them towards becoming independent researchers and scholars.

Dr. S. Gunasekaran
Dean, Research and Development

GUIDELINES FOR THE PREPARATION OF SYNOPSIS AND Ph.D. THESIS

1 General

The manual is intended to provide broad guidelines to the research scholars in the preparation of the Ph.D. Thesis. In general, a thesis shall report, in an organized and scholarly fashion, an account of original research work of the research scholar leading to the discovery of new facts or techniques or correlation of facts already known (analytical, experimental, hardware oriented, etc.). Thesis shall demonstrate a quality as to make a definite contribution to the advancement of knowledge and the research scholar's ability to undertake sustained research and present the findings in an appropriate manner with actual accomplishments of the work.

The scholars are advised to read carefully the instructions given in the sequel and meticulously follow them in the preparation of thesis. Non-compliance with any of these instructions may lead to the rejection of the thesis submitted.

2 Size of thesis

The size of the thesis should be minimum 150 pages (in case of mathematics, minimum 100 pages) and maximum 300 pages of typed matter reckoned from the first page of Chapter 1 to the last page of the thesis excluding reference section, Tables and Figures. Under extraordinary circumstances, the size of the thesis shall be permitted up to 400 pages with the concurrence of the supervisor.

3 Arrangement of the contents of the thesis

The thesis material should be arranged and bound in the following sequence. The heading for each section should be formatted in Times New Roman font, size 15.

- (i) *Cover Page and Title page*
- (ii) *Certificate given by the Supervisor*
- (iii) *Declaration Certificate by the candidate*
- (iv) *Acknowledgement by the Candidate*
- (v) *Contents*
- (vi) *Abstract (Papers published in Journals and papers presented in Conferences)*
- (vii) *List of Tables*
- (viii) *List of Figures*
- (ix) *List of Abbreviations and Symbols*
- (x) *Chapters*
- (xi) *References*
- (xii) *Annexures*

The Tables and Figures should be included at appropriate places in the text of the Thesis.

4 Page Dimensions and Margin

Standard A4 Size (297 mm x 210 mm) paper may be used for preparing the copies. The dimensions of the final bound thesis (4 copies) report should be 290 mm x 205 mm. Thesis should be bound with flexible cover of thick white art paper.

The final thesis (at the time of submission) should have the following page margins:

Top edge : 30 to 35 mm or 1.38 inches

Bottom edge : 25 to 30 mm or 1.18 inches

Left side : 35 to 40 mm or 1.57 inches

Right side : 20 to 25 mm or 0.98 inches

The Thesis should be prepared on good quality white paper preferably not lower than 80gsm. Tables and Figures should conform to the margin specifications. Large size Figures should be photographically or otherwise reduced to the appropriate size before insertion.

5 Manuscript Preparation

In the preparation of the manuscript, care should be taken to ensure that all textual matter is typewritten to the extent possible in the same format as may be required for the final thesis. Hence some of the information required for the final typing of the thesis is also included in this section.

The headings of all items from (ii) to (v) listed in section 3 should be typed in capital letters and heading of all items from (vi) to (ix) should be typed in sentence case without punctuation and centered 50 mm below the top of the page. The text should commence 4 spaces below this heading. The page numbering for all items from (iii) to (ix) should be done using lower case Roman numerals and the pages thereafter should be numbered using Arabic numerals.

5.1 Cover Page & Title Page

A specimen copy of the Cover page and Title page for the Thesis is given in **Annexure I**.

5.2 Certificate

The Certificate shall be typed in double line spacing using Font style Times New Roman and Font Size 13 as per the format shown in **Annexure II**.

5.3 Declaration

Declaration certificate, as given in the specimen in **Annexure III** is to be given by the candidates with the counter signature by the supervisor. The certificate shall carry the Supervisor's signature and shall be followed by the **Supervisor's name, academic designation (not any other responsibilities of administrative nature)**, department and full address of the institution where the supervisor has guided the research scholar. The term 'SUPERVISOR' must be typed in capital letters below the supervisor's name. Signature of the Joint Supervisor with the details specified as above should be included wherever it is applicable.

5.4 Acknowledgement

It should be brief and should not exceed two pages when typed in **double spacing**. The scholar's signature shall be made at the bottom right end above his/her name typed in capitals.

5.5 Table of Contents

The table of contents should list all captions following it as well as any caption which precedes it. The title page, Certificate, Declaration and Acknowledgment will not find

a place among the items listed in the Table of Contents but the page numbers of which are in lower case Roman letters. One and a half spacing should be adopted for typing the matter under this head. A specimen copy of the table contents for the thesis is given in **Annexure IV**.

5.6 Abstract

Abstract should be an essay type of narration not exceeding four pages outlining the research problem, methodology used for tackling it and a summary of the findings. This shall be typed in **double line** spacing using Font Style Times New Roman and Font Size 13, including the list of publications and list of paper presentations in conferences as given in **Annexure V**

5.7 List of Tables

The list should use exactly the same captions as they appear above the tables in the text. One and half spacing should be adopted for typing matter under this head. A Specimen copy of the list of Tables is given in **Annexure VI**.

5.8 List of Figures

The list should use exactly the same captions as they appear below the figures in the text. One and a half spacing should be adopted for typing the matter under this head. A Specimen copy of the list of Figures is given in **Annexure VII**.

5.9 List of Abbreviations and Symbols

One and a half spacing should be adopted for typing the matter under this head. Standard symbols, abbreviations, etc. should be used. The list should be arranged alphabetically with respect to the contents on the right side as shown in **Annexure VIII**.

5.10 Chapters

The chapters may be broadly divided into 3 parts, (i) introductory chapter, (ii) chapters developing the main theme of the thesis (like review, investigations conducted) and (iii) results, discussion and conclusion. The main text shall be divided into several chapters and each chapter may be further divided into several divisions and sub-divisions. Each chapter should be given an appropriate title.

Tables and Figures in a chapter should be placed in the immediate vicinity of the reference where they are cited.

Footnotes should be used sparingly. They should be typed single space and placed directly underneath in the very same page which refers to the material they annotate.

5.11 Annexures

Annexures are provided to give supplementary information, which if included in the main text may serve as a distraction and cloud the central theme under discussion. Annexures should be numbered using Arabic numerals, e.g. Annexure 1, Annexure 2, etc.

5.12 List of References

Any works of other researchers, if used either directly or indirectly, the origin of the material thus referred to at appropriate places in the Thesis should be indicated.

The author's publications during the period of research should not be included in the references and can be separately mentioned as in 5.10. A paper, a monograph or a book may be designated by the name of the first author followed by the year of publication, placed inside brackets at the appropriate places in the Thesis. The citation may assume any one of the following forms.

Examples of Citation

- (i) An improved algorithm has been adopted in the literature (**Wilson, 2009**)
- (ii) **Massey and Mittelholzer (2008)** have dealt at length this principle
- (iii) The mechanical manipulators has been studied by **Anigstein et al., (2010)** and certain limitations of the method used, has been pointed out by **Anigstein et al., (2010)**.
- (iv) **Anwar Shahawy et al., (2016)** have discussed the DFT quantum spectroscopic studies on the anti-cancer effect of Ibuprofen drug.

The listing should be typed 4 spaces below the heading "REFERENCES" in single spacing. The reference material should be listed in the alphabetical order of the first author. The name of the author/authors should be immediately followed by the other details and year. A typical illustrative list given below relates to the citation example quoted above.

References

- [1] **Alishahi, K., Marvasti, F., Aref, V. and Pad, P.**, "Bounds on the sum capacity of synchronous binary CDMA channels", Journal of Atmosphere Chemical Society, Vol. 55, No. 8, pp.3577- 3593, 2010.
- [2] **Capocelli, R., De Santis, A. and Vaccano, U.**, "Eds. Springer-Verlag, New York", 2007.
- [3] **Djionin, D. and Bhagrava, V.**, "New results on low complexity detectors for over-saturated CDMA systems" Proceedings of Globecom, 2010.
- [4] **Karystinos, G. N. and Pados, D. A.**, "The maximum squared correlation, total asymptotic efficiency, and sum capacity of minimum total squared correlation binary signature sets", Designs, Codes and Cryptography, Vol. 51, pp. 348-355, 2007.
- [5] **Massey, J. L. and Mittelholzer, T.**, "Welch's bound and sequence sets for code-division multiple access systems", Sequences II, Methods in Communication, Security and Computer Sciences",
- [6] **Verdu, S.**, "Multiuser Detection", Cambridge University Press, New York, 2008.
- [7] **Waldron, S.**, "Generalized Welch bound equality sequences are tight frames", IEEE Transaction Information Theory, Vol. 49, No. 9, pp. 2307-2309, 2008.

5.13 Tables and Figures

"Table" means tabulated numerical data in the body of the thesis as well as in the appendices. All other non-verbal material used in the body of the thesis and appendices such as charts, graphs, maps, photographs and diagrams may be designated as Figures.

A Table or Figure including caption should be accommodated within the prescribed margin limits and appear on the page following the page where their first reference is made. Tables and Figures on half page or less in length may appear on the same page along with the text. However, they should be separated from the text both above and below by triple spacing.

All Tables and Figures should be prepared on the same paper or material used for the preparation of the rest of the thesis. Two or more small Tables or Figures may be grouped if necessary in a single page. Wherever possible, the photograph(s) shall be reproduced on a full sheet of photographic paper or color Xerox. More than one photograph can be included in a page. Samples of Fabric, Leather, etc., if absolutely necessary may be attached evenly

Tables and Figures shall be presented as per the format shown in **Annexure IX**.

6 Typing Instructions

6.1 General

This section includes additional information for final typing of the Thesis. The impressions on the typed/Xeroxed/printed copies should be in black toner.

A sub-heading at the bottom of a page must have at least two full lines below it or else it should be carried over to the next page.

The last word of any page should not be split using a hyphen. One and a half spacing should be used for typing the general text. The general text shall be typed in Font Style Times New Roman and Font Size 13. Single spacing should be used for typing:

- (i) Long Tables
- (ii) Long quotations
- (iii) Foot notes
- (iv) Multiline captions
- (v) References

All quotations exceeding one line should be typed in an indented space - the indentation being 15 mm from either side of the margin.

6.2 Chapters

The format for typing Chapter headings, Division headings and Sub-division headings are explained by the following illustrative examples.

Chapter heading	:CHAPTER 1
	Introduction (Caption of the chapter)
Division heading	:1.1 Outline of Thesis
Sub-division heading	:1.1.1 Literature Review
	<i>1.1.1.1 Synthetic aperture radars on satellites</i>

The word CHAPTER without punctuation should be centered 50 mm down from the top of the page. Two spaces below, the title of the chapter should be typed centrally in sentence case. The text should commence 4 spaces below this title, the first letter of the text starting 20 mm inside from the left hand margin.

The division and sub-division captions along with their numberings should be left justified. The typed material directly below division or sub-division heading should commence 2 spaces below it and should be offset 20 mm from the left hand margin. Within a division or sub-division paragraphs are permitted. Even paragraph should commence 3 spaces below the last line of the preceding paragraph, the first letter in the paragraph being offset from the left hand margin by 20 mm.

7 Numbering Instructions

7.1 Page Numbering

All page numbers (whether it is in Roman or Arabic numbers) should be typed without punctuation on the upper right hand corner 20 mm from the top with the last digit in line with the right hand margin. The preliminary pages of the thesis (such as Certificate, Declaration, Acknowledgement, Table of Contents, Abstract, List of Tables, List of Figures and List of Symbols and Abbreviations) should be numbered in lower case Roman numerals. The Certificate page will be numbered as (i) but this should not be typed till last page of the Table of Contents. The page after the Table of Contents i.e. Abstract shall be numbered with continuous numbering starting from the Certificate page and it should appear at the top right hand corner as already specified. Pages of main text, starting with Chapter 1 should be consecutively numbered using Arabic numerals.

7.2 Numbering of Chapters, Divisions and Sub-Divisions

The numbering of chapters, divisions and sub-divisions should be done using Arabic numerals only and further decimal notation should be used for numbering the divisions and sub-divisions within a chapter. For example, sub-division 4 under division 3 belonging to chapter 2 should be numbered as 2.3.4. The caption for the sub-division should immediately follow the number assigned to it with one space.

Every chapter beginning with the first chapter should be serially numbered using Arabic numerals. Appendices, included if any, should also be numbered in an identical manner starting with Appendix 1.

7.3 Numbering of Tables and Figures

Tables and Figures appearing anywhere in the thesis should bear appropriate numbers. The rule for assigning such numbers is illustrated by an example. Thus, if a Fig. in Chapter 3 happens to be the fourth then assign 3.4 to that Fig. Identical rules apply for Tables except that the word Fig. is replaced by the word Table. If Figures (or Tables) appear in appendices then **Fig. 3** in chapter 2 will be designated as **Fig. 2.3**. If a table to be continued into the next page this may be done, but no line should be drawn underneath an unfinished Table. The top line of the Table continued into the next page should, for example read **Table 2.1** (continued) placed centrally and underlined. Tables and Figures shall be included (in bold) in the text, in the appropriate places.

7.4 Numbering of Equations

Equations appearing in each Chapter or Appendix should be numbered serially, the numbering should commence afresh for each Chapter or Appendix. Thus for example, an equation appearing in chapter 4, if it happens to be the eighth equation in that chapter should be numbered as (4.8) thus:

$$Y = ax^2 + bx + C \quad (4.8)$$

While referring to this equation in the body of the Thesis it should be referred to as Equation (4.8).

Note:

- 1. The acceptable limit of plagiarism percentage of the thesis is up to 10% in Anti-Plagiarism web tool as per UGC guidelines.**
- 2. The grammar report of the thesis shall be with 0% errors.**

ANNEXURE I

A typical Specimen of Cover Page and Title Page

(“Title of the Thesis”)

 <1.5 line spacing>

THESIS

Submitted to

**St. PETER’S INSTITUTE OF HIGHER EDUCATION AND
RESEARCH**

in partial fulfillment of the requirements for the award of the degree of

 <Italic> <1.5 line spacing>

DOCTOR OF PHILOSOPHY

IN

.....
(Name of the Department)

By

.....
(Name of the Candidate)

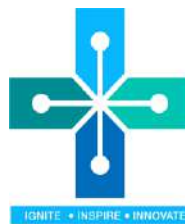
(Regn. No.....)

 <1.5 line spacing>

Under the guidance of

(Name of the Supervisor)

 <1.5 line spacing>



DEPARTMENT OF -----

St. PETER’S INSTITUTE OF HIGHER EDUCATION AND RESEARCH

(Deemed to be University U/S 3 of the UGC Act, 1956)

AVADI, CHENNAI - 600 054

<1.5 line spacing>

(Month Year)

ANNEXURE II

CERTIFICATE

I certify that the thesis entitled, “**Spectroscopic and Quantum Chemical Calculations of some Antiepileptic Drugs**” submitted for the degree of Doctor of Philosophy (Ph.D.) by is the record of research work carried out by her during the period 2012-2015 under my guidance and supervision, and that this thesis has not formed the basis for the award of any Degree, Diploma, Associateship, Fellowship or other Titles in this institution or any other institution of Higher Learning.

Place:
(Signature of the Supervisor)
Date
(Name of the Supervisor)
SUPERVISOR
(with seal)

DECLARATION

I declare that the thesis entitled “**Spectroscopic and Quantum Chemical Calculations of some Antiepileptic Drugs**” submitted by me for the degree of Doctor of Philosophy (Ph.D.) is the record of work carried out by me during the period 2012-2015 under the guidance of and has not formed the basis for the award of any Degree, Diploma, Associate ship, Fellowship, Titles in this institution or any other institution or other similar institution of Higher Learning.

.....
(Signature of the Supervisor)

.....
(Name of the Supervisor)

SUPERVISOR
(with seal)

.....
(Signature of the Research Scholar)

.....
(Name of the Scholar)

.....
(Department)

Place:

Date:

CONTENTS

Chapter	Title	Page
	Abstract	iv
	List of Tables	vi
	List of Figures	vii
	List of Abbreviations and Symbols	viii
1	Anti-Epileptic Drugs – An Overview	1
1.1	Introduction	1
1.2	Causes for Epilepsy	3
1.3	Types of Epilepsy	4
1.4	Antiepileptic Drug	6
1.5	Metabolic Agents	9
1.6	Conclusion	10
2	Instrumentation Techniques	19
2.1	Introduction	19
2.1.1	Proposed Method	20
2.1.2	Results and Discussion	20
2.2	Fourier Transform Infrared Spectral Analysis	22
2.3	Fourier Transform Raman Analysis	24
2.4	UV-Visible Spectroscopy	26
2.5	NMR Spectroscopy	28
3	Theory of Quantum Chemical Methods	38
3.1	Introduction	38
3.1.1	Prevention and Counter Measures	39
3.1.2	Fountain Codes	40
3.1.3	Encoding Process of Fountain Codes	41
3.1.4	Decoding Process of Fountain Codes	41
3.1.5	Advantages	43
3.1.6	Disadvantages	44
3.2	Ab-initio Method	45

Chapter	Title	Page
4	Molecular Structure, Spectroscopic Characterization of Levetiracetam based on Quantum Chemical Calculations	48
4.1	Introduction	48
4.2	Experimental Methods	49
4.3	Quantum Chemical Calculations	50
4.4	Conclusion	50
5	Quantum Chemical Study on Vibrational, Electronic Transitions, OMO-LUMO and NMR Analysis of Pregabalin	85
5.1	Introduction	85
5.2	Experimental Methods	87
5.3	Computational Details	88
5.4	Conclusion	89
6	Density Functional Theory, Restricted Hartree-Fock Simulations and FTIR, FT-Raman Studies on Gabapentin	110
6.1	Introduction	111
6.2	Experimental Details	112
6.3	Quantum Chemical Calculations	113
6.4	Conclusion	115
7	Computation and Interpretation of Vibrational Spectra of Lacosamide using Ab-initio and Density Functional Methods	138
7.1	Introduction	139
7.2	Experimental Methods	139
7.3	Computational Details	142
7.4	Conclusion	143
8	Ab-initio and Density Functional Theory Studies of Vibrational Spectra and Assignment of Fundamental Modes of Acetazolamide	167
8.1	Introduction	167
8.2	Experimental Details	168
8.3	Quantum Chemical Calculations	169
8.4	Conclusion	170
9	Structural and Qualitative Studies on Lamotrigine	191
9.1	Introduction	191
9.1.1	Personal Health Record	192
9.1.2	Electronic Medical Record System	194
9.1.3	Electronic Health Record (EHR)	195

Chapter	Title	Page
9.2	Experimental Methods	196
9.3	Qualitative Analysis	197
9.4	Computational Details	198
9.5	Conclusion	199
10	Conclusion and Scope for Further Study	216
10.1	Conclusion	216
10.2	Scope for Further Study	217
	References	222

ANNEXURE V

A part of the material of the thesis has been published in reputed Journals /presented in Conferences.

(a) Journals

- [1] **Manimaran, A. and Somasundaram, K.**, “An Optimized Core Aided Mesh Protocol for MANET Multicasting”, International Journal of Applied Engineering Research (IJAER), Vol. 10, No. 5, pp. 13437-13446, 2015.
- [2] **Manimaran, A. and Somasundaram, K.**, “AMRA: Angle based Multicast Routing Algorithm for Wireless Mesh Networks”, Indian Journal of Science and Technology, Vol. 8, No. 13, pp. 1-8, 2015.

(b) Conferences

- [1] **Manimaran, A. and Somasundaram, K.**, “FTIR, FT-Raman Spectra and DFT Calculation of Levetiracetam”, Proceedings of Inter National Conference on Research in Condensed Matter Physics (ICCMP), October 1-3, 2012.
- [2] **Manimaran, A. and Somasundaram, K.**, “FTIR, FT-Raman Spectra and Quantum Chemical Calculation of (S)-2- (Oxopyrrolidin-1-yl) Butanamide”, Proceedings of International Conference on Recent Advances in Physics (ICRAP), August 12-13, 2013.

ANNEXURE VI

List of Tables

Table	Title	Page
1.1	Chemical name and Structure of some Antiepileptic drugs	13
1.2	Physio-Chemical details of Antiepileptic drugs taken under study	15
4.1	Bond lengths (A^0) of Levetiracetam	52
4.2	Bond angles (0) of Levetiracetam	53
4.3	Calculated and Experimental wave numbers (cm^{-1}) of Levetiracetam	58
4.4	Mulliken and Natural Atomic charges of Levetiracetam	66
4.5	The calculated ^{13}C and ^1H NMR chemical shifts of Levetiracetam	71
4.6	Assignment of observed electronic transitions of Levetiracetam	73
4.7	Comparison of HOMO, LUMO, energy gap and related global quantities of Levetiracetam	76
4.8	Condensed Fukui functions and local softness of Levetiracetam	78
4.9	The calculated and components of Levetiracetam	79
4.10	Thermodynamic parameter of Levetiracetam	82
4.11	Thermodynamic parameter of Levetiracetam at different temperatures	83
5.1	Bond lengths (A^0) for Pregabalin	90
5.2	Selected bond angles (0) for Pregabalin	91
5.3	Calculated and Experimental wave numbers (cm^{-1}) for Pregabalin	95
5.4	Mulliken and Natural Atomic charges of Pregabalin	100
5.5	Assignment of observed electronic transitions of Pregabalin	101
5.6	The calculated ^{13}C and ^1H NMR chemical shifts of Pregabalin	105
5.7	Thermodynamic properties of Pregabalin	108

Table	Title	Page
8.8	Thermodynamic parameter of Acetazolamide	189
9.1	Absorbance for certain modes of vibration under different conditions of storage for Lamotrigine	195
9.2	Internal Standard Evaluation for Lamotrigine	196
9.3	Lamotrigine stored at different conditions	199
9.4	Selected optimized geometrical parameters of Lamotrigine	202
9.5	Mulliken and Natural Atomic charges of Lamotrigine	204
9.6	Vibrational wave numbers(cm^{-1}) obtained for Lamotrigine by FTIR, FT Raman; reduced mass; force constant; IR intensity by RHF and B3LYP/6-311++G(d,p)levels	207
9.7	Thermodynamic properties of Lamotrigine at room temperature	214
9.8	Thermodynamic properties of Lamotrigine at different temperature	214

ANNEXURE VII

List of Figures

Figure	Title	Page
2.1	Optical path diagram of FTIR Spectrometer	26
2.2	Spectrum One : FTIR Spectrometer	26
2.3	Optical path diagram of FT- Raman Spectrophotometer	28
2.4	BRUKER RFS 27: Stand alone FT-Raman Spectrophotometer	28
2.5	Optical path diagram of UV- Visible Spectrophotometer	33
2.6	Cary 5E UV-Vis Spectrophotometer	33
4.1	Atom numbering of Levetiracetam	52
4.2	FTIR spectrum of Levetiracetam	56
4.3	FT- Raman spectrum of Levetiracetam	56
4.4	Graphical representation of Natural charge distribution of Levetiracetam	64
4.5	HOMO and LUMO energy structure of Levetiracetam	68
4.6	Two dimensional Contour map of Levetiracetam	68
4.7	H NMR spectrum of Levetiracetam (Experimental,B3PW91,B3LYP/6-311++G(d,p))	69
4.8	C NMR spectrum of Levetiracetam (Experimental, B3PW91,B3LYP/6-311++G(d,p))	69
4.9	UV – Vis Spectrum of Levetiracetam	73
4.10	Thermodynamic functions graph of Levetiracetam	81
5.1	Atom numbering scheme of Pregabalin	89
5.2	FTIR spectrum of Pregabalin	92
5.3	FT-Raman spectrum of Pregabalin	92
5.4	HOMO and LUMO energy structure of Pregabalin	98
5.5	Graphical representation of Mulliken and Natural charge distribution of Pregabalin	99
5.6	H NMR spectrum of Pregabalin	103
5.7	C NMR spectrum of Pregabalin	103

Figure	Title	Page
5.8	Experimental H NMR spectrum of Pregabalin	104
5.9	Experimental C NMR spectrum of Pregabalin	104
5.10	Thermodynamic functions graph of Pregabalin	109
6.1	Atom numbering scheme of Gabapentin	114
6.2	FTIR spectrum of Gabapentin	118
6.3	FT-Raman spectrum of Gabapentin	118
6.4	NPA plot of Gabapentin	128
6.5	Variation of Thermodynamic parameter with Temperature	137
7.1	Atom numbering of Lacosamide	142
7.2	FTIR spectrum of Lacosamide	146
7.3	FT-Raman spectrum of Lacosamide	146
7.4	Graphical representation of Natural charge distribution of Lacosamide	159
7.5	UV-Vis spectrum of Lacosamide	160
8.1	Atom numbering of Acetazolamide	171
8.2	FTIR spectrum of Acetazolamide	174
8.3	FT- Raman spectrum of Acetazolamide	174
8.4	HOMO and LUMO energy structure of Acetazolamide	183
8.5	Molecular Electrostatic Potential spectrum of Acetazolamide	185
9.1	Overlay spectrum of Lamotrigine stored at different Condition	194
9.2	UV-Vis spectrum of Lamotrigine	199
9.3	Atom numbering scheme of Lamotrigine	201
9.4	3D plots of HOMO and LUMO of Lamotrigine	203
9.5	FTIR spectrum of Lamotrigine	206
9.6	FT-Raman spectrum of Lamotrigine	206
9.7	Thermodynamic graph of Lamotrigine at different Temperature	215

ANNEXURE VIII

List of Abbreviations and Symbols

API	-	Active Pharmaceutical Ingredient
ALLHAT	-	The Antihypertensive and Lipid-Lowering Treatment to Prevent Heart Attack Trial
AMI	-	Austin Model 1
APD	-	Avalanche Photodiode
ARB	-	Angiotensin II Receptor Blocker
AT1	-	Angiotensin II Receptor Blocker type I
ATR	-	Attenuated Total Reflection
B3LYP	-	Becke-3-Lee-Yang-Parr
CW	-	Continuous Wave
DFT	-	Density Functional Theory
ESR	-	Electron Spin Resonance
FDA	-	Food and Drug administration
FTIR	-	Fourier Transform Infra-Red
HBP	-	High blood pressure
HF	-	Hartree-Fock
HOMO	-	Highest Occupied Molecular Orbital
HTN or HT	-	Hypertension
HYD	-	Hydrochlorothiazide
ICH	-	International Council on Harmonisation
JNC	-	Joint National Committee
LIFE	-	Losartan Intervention for Endpoint Reduction
LOS	-	Losartan
LUMO	-	Lower Unoccupied Molecular Orbital
\bar{r}	-	Average rating
ΣJ_i	-	Cost Function
$\omega ()$	-	Large Quantity In Higher Order
v_p	-	Product Embedding
τ	-	Radius
α	-	Updating Parameter

ANNEXURE IX

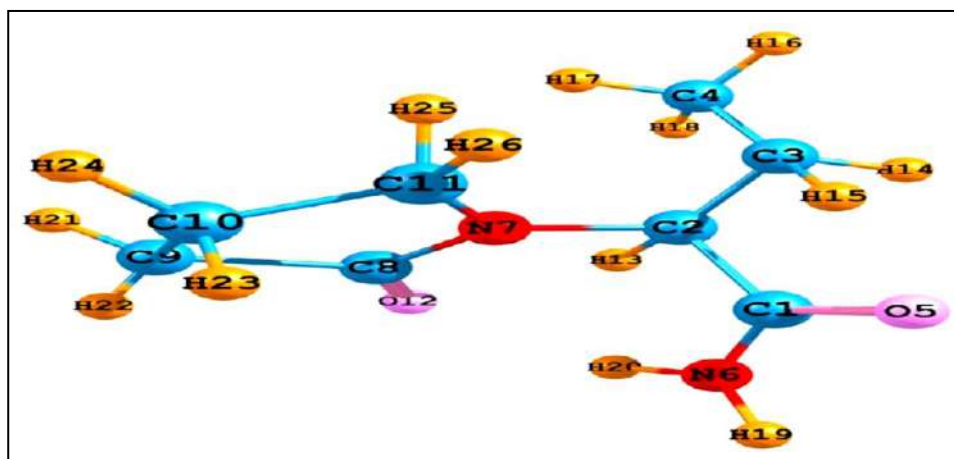


Fig. 4.1 Optimised geometric structure and numbering of atoms of Levetiracetam

Table 4.1 Bond parameters of Levetiracetam with different basis sets, RHF/6-311++G (d, p), B3WP91/6-311++ (d, p), B3LYP/6-311++(d, p)

Parameter	Method/basis set			Lit. value
	RHF/6-311++G(d,p)	B3WP91/6-311++G(d,p)	B3LYP/6-311++G(d,p)	
C ₁ -C ₂	1.531	1.542	1.546	1.530
C ₁ -O ₅	1.200	1.222	1.224	1.240
C ₁ -N ₆	1.349	1.358	1.362	1.319
C ₂ -C ₃	1.526	1.524	1.529	1.530
C ₂ -C ₇	1.457	1.460	1.467	1.460
C ₂ -H ₁₃	1.082	1.096	1.095	1.094
C ₃ -C ₄	1.527	1.525	1.531	1.530
C ₃ -H ₁₄	1.085	1.095	1.095	1.094
C ₄ -H ₁₅	1.083	1.095	1.094	1.094
C ₄ -H ₁₆	1.085	1.094	1.094	1.094
C ₄ -H ₁₇	1.085	1.094	1.095	1.094
C ₄ -H ₁₈	1.086	1.095	1.095	1.094
N ₆ -H ₁₉	0.993	1.008	1.009	1.014
N ₆ -H ₂₀	0.995	1.014	1.014	1.046
N ₇ -C ₈	1.351	1.362	1.366	1.320
N ₇ -C ₁₁	1.456	1.456	1.464	1.470
C ₈ -C ₉	1.514	1.520	1.525	1.510
C ₈ -O ₁₂	1.203	1.228	1.229	1.230
C ₉ -C ₁₀	1.531	1.532	1.538	1.541
C ₉ -H ₂₁	1.086	1.097	1.096	1.094
C ₉ -H ₂₂	1.081	1.092	1.091	1.091
C ₁₀ -C ₁₁	1.538	1.541	1.547	1.530
C ₁₀ -H ₂₃	1.084	1.094	1.094	1.094
C ₁₀ -H ₂₄	1.082	1.093	1.092	1.094
C ₁₁ -H ₂₅	1.086	1.098	1.097	1.094