**Curriculum Vitae**



**Name**                       : **Dr.P.Gayathri**

**Designation**              : Assistant Professor (SG)

**Department**            : Physics

**Area of interest**        :            Crystal growth and structure determination-Crystallography and molecular spectroscopy

**Institution :** Periyar Maniammai Institute of Science and Technology

**Academic Background :**

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| **Sno** | **Teaching Experience** | **Research Experience** |
| 1. | 15 | 7 years |

**Awards received**      :      **Received ISTE 2011 National Award for the best research work  done below 35 years.**

**Project Guided:**

**Ph.D Guided : 03**

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| **S.no** | **Name of the scholar** | **Title of thesis** | **Completion** |
| 1 | A.Madanagopal | Pharamaco dynamic activity analysis and structural property interpretation on some anitibiotic compounds | December2018 |
| 2 | D.Shoba | Quantum Computational (HF/DFT) and experiments spectral analysis of certain biologically and pharmacentically important molecules  | October 2015 |
|  3 | A.Suvitha  | An experimental and theoretical (HF/DFT) investigation of certain biomedically active compounds | November 2015 |

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| Sno | Course | Title of the project |
| 1. | **M. Phil** | Growth & characterization of Nickel Sulphate doped with EDTA |
| 2.  | **M.Tech** | Photoluminescence study of cdTe/cdSe quantum Dots for Solar Cell applications |

**Research Area : X- Ray Crystallography**

**Application of the research work.**

**X-ray crystallography** is a method of determining the arrangement of atoms within a crystal, in which a beam of X-rays strikes a crystal and diffracts into many specific directions. From the angles and intensities of these diffracted beams, a crystallographer can produce a three-dimensional representation of the density of electrons within the crystal. From this electron density, the mean positions of the atoms in the crystal can be determined, as well as their chemical bonds, their disorder and various other information.

X – ray crystal structures can also account for unusual electronic or elastic properties of a material, shed light on chemical interactions and processes, or serve as the basis for designing pharmaceuticals against diseases.

As part of our research work we have analysed crystal and molecular structure of some substituted Piperidine and Imidazole derivatives by single crystal X-ray diffraction.

Piperidones are an important group of heterocyclic compounds in the field of medicinal chemistry due to their biological activities, including cytotoxic and anticancer properties. The importance of piperidine and imidazole are given below.

Piperidones were also reported to possess analgesic, anti-inflammatory, central nervous system CNS, local anaesthetic, anticancer and antimicrobial activity. The design and synthesis of conformationally anchored molecules is an important approach towards improving potency and selectivity. The Pharmacological effects of potential drugs depend sensitively on the stereochemistry and ring conformations.

Imidazole derivatives have been used to construct highly sensitive fluorescent chemisensors for sensing and imaging of metal ions and its chelates in particular those with Ir3+ are major components for organic light emitting diodes and are promising candidates for fluorescent chemisensors for metal ions.

**Journals Publication – International**

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| S.No | Title of the paper | Author Name | Journal Name | Year of publication |
| 1. | 4,5-Dimethyl-2-phenyl-1-(p-tolyl)-1H-imidazole | P. Gayathri, A. Thiruvalluvar, N. Srinivasan, J. Jayabharathi and R. J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2010). E**66**, o2826 |
| 2 | 2-(4-Fluorophenyl)-1-(4-methoxyphenyl)-4,5-dimethyl-1Himidazole | P. Gayathri, J. Jayabharathi, K. Saravanan, A. Thiruvalluvar and R.J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2010). E**66**, o1791 |
| 3 | 2-(4-Fluorophenyl)-4,5-dimethyl-1-(4-methylphenyl)-1Himidazole | P. Gayathri, J. Jayabharathi, N. Srinivasan, A. Thiruvalluvar and R. J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2010). E**66**, o1703 |
| 4. | 4,5-Dimethyl-1,2-diphenyl-1H-imidazole monohydrate | P. Gayathri, A. Thiruvalluvar, K. Saravanan, J. Jayabharathi and R. J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2010). E**66**, o2219 |
| 5. | 2-(4-Fluorophenyl)-1,4,5-triphenyl-1H-imidazole | P. Gayathri, A. Thiruvalluvar, N. Srinivasan, J. Jayabharathi and R. J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2010). E**66**, o2519 |
| 6. | 1-(3,5-Dimethylphenyl)-4,5-dimethyl-2-phenyl-1H-imidazolehemihydrate | P. Gayathri, A. Thiruvalluvar, N. Srinivasan, J. Jayabharathi and R. J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2010). E**66**, o2776 |
| 7. | 1-Benzyl-3,5-bis[(E )-3-thienylmethylidene]piperidin-4-one | P. Gayathri, A. Thiruvalluvar, K. Rajeswari, K. Pandiarajan and R. J. Butcher | Acta Crystallographica Section E | Acta Cryst. (2011). E**67**, o571 |
| 8. | t -3-Pentyl-r -2,c-6-diphenylpiperidin-4-one | P. Gayathri, J. Jayabharathi, G. Rajarajan, A. Thiruvalluvar and R. J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2009). E**65**, o3083 |
| 9. | r -2,c-6-Bis(4-chlorophenyl)-t -3-isopropyl-1-nitrosopiperidin-4-one | P. Gayathri, A. Thiruvalluvar, A. Manimekalai, S. Sivakumar and R. J.Butcher | Acta Crystallographica Section E | Acta Cryst. (2008). E**64**, o1973 |
| 10. | 1-Methyl-3,5-bis[(E )-(3-methyl-2-thienyl)methylene]piperidin-4-onemonohydrate | K. Rajeswari, K. Pandiarajan, P. Gayathri and A. Thiruvalluvar | Acta Crystallographica Section E | Acta Cryst. (2009). E**65**, o885 |
| 11. | 1-Formyl-r -2,c-6-bis(4-methoxyphenyl)-t -3-methylpiperidin-4-one | P. Gayathri, P. Sakthivel, S. Ponnuswamy, A. Thiruvalluvar and R. J. Butcher | Acta Crystallographica Section E | Acta Cryst. (2009). E**65**, o2813 |
| 12. | r-2,c-6-Bis(4-methoxyphenyl)-c-3,t-3-dimethylpiperidin-4-one | S. Ponnuswamy,a V. Mohanraj, P. Gayathri,A. Thiruvalluvar and R. J. Butcher | Acta Crystallographica Section E | Acta Cryst. (2008). E64, o2328 |
| 13. | r -2,c-6-Bis(4-chlorophenyl)-c-3,t -3-dimethylpiperidin-4-one | S. S. Ilango, S. Ponnuswamy, P. Gayathri, A. Thiruvalluvar and R. J. Butcher | Acta Crystallographica Section E | Acta Cryst. (2008). E**64**, o2312 |
| 14. | 3,3-Dimethyl-cis-2,6-di-p-tolylpiperidin-4-one | P. Gayathri, S. S. Ilango, S. Ponnuswamy, A. Thiruvalluvar and R. J. Butcher | Acta Crystallographica Section E | Acta Cryst. (2009). E**65**, o2445 |
| 15. | (E )-N*\_*-(3,3-Dimethyl-2,6-diphenylpiperidin-4-ylidene)isonicotinohydrazide | C. Sankar, K. Pandiarajan, A. Thiruvalluvar and P. Gayathri | Acta Crystallographica Section E | Acta Cryst. (2010). E**66**, o2841 |

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| **S.No** | **Title of the paper** | **Journal** **Name**  | **Indexed in** | **Impact Factor** | **ISSN No./Vol. No./Issue No./ Pg.No.** | **Month & year of publication** | **Type of Journal (International /National/Local)** |
| **1** | Spectroscopic and computational investigation of the structure and pharmacological activity of 1-benzylimidazole | Journal of Taibah university of scienceElsevier | science direct | 2.40 | Received 5 November 2016;  | accepted 18 February 2017(975-996) | International |
| **2** | Molecular structure activity on pharmaceutical applications of Phenacetin using spectroscopic investigation | Journal of Molecular StructureElsevier | Scopus/Google scholar (Non-paid) | 1.602 | Journal of Molecular Structure 1127 (2017) 611-625 | 13th Aug 2016 | International  |
| **3** | Vibrational analysis using FT-IR, FT-Raman spectra and HF–DFT methodsand NBO, NLO, NMR, HOMO–LUMO, UV and electronic transitions studies on 2,2,4-trimethyl pentane | **Spectrochimica** Acta Part A: Molecular and Biomolecular SpectroscopyElsevier | Scopus/Google scholar (Non-paid) | 2.098 | 138 (2015) 900–912 | 2015 | International |
| **4** | Quantum mechanical and spectroscopic (FTIR, FT-RAMAN,NMR AND UV) Study On The Structure, Polarizability,Nbo Analysis of 1-Bromo-4-Merhyl Naphthalene | Journal of Advanced Science & Engineering  | Scopus/Google scholar (Non-paid) | 2.098 | 2015 | 2015 | International |
| **5** | NBO, HOMO–LUMO, UV, NLO, NMR and vibrational analysis of veratroleusing FT-IR, FT-Raman, FT-NMR spectra and HF–DFT computational mtd | Spectrochimica Acta Part A: Molecular and Biomolecular SpectroscopyElsevier | Scopus/Google scholar (Non-paid) | 2.098 | 138 (2015) 357–369 | 2015 | International |
| **6.** | Vibrational and NMR Investigation on Pharmaceutical Activity of 2,5-Dimethoxy-4-Ethylamphetamine by Theoretical and Experimental Support | **Journal of Molecular Pharmaceutics****and Organic Process Research** | Scopus/Google scholar (Non-paid) |  | **Received Date**: January 31, 2017, **Accepted Date**: February 28, 2017,  | **Published Date**: March 07, 2017 | International |
| **7.** | Vibrational spectra (FT-IR and FT-Raman) and computed DFT analysis of Isonicotinic acid 2 methyl ester Spectrochimica | **Acta Part A:molecular and Biomolecular spectroscopy spectrochimica ,Acta part A: Molecular and Biomolecular spectroscopy** | Scopus/Google scholar (Non-paid) |  | **136(2015)****852-863** | **2015** | Interational |

**Book Publication:**

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| **Title** | **Publisher &Year** |
| Applied Physics for First semester B.Tech students with ISBN number (978-81-920465-3-2) | Periyar Maniammai University & 2011 |

**Membership in Professional Bodies :**

* + - * 1. Life membership for Indian Society for Technical Education (ISTE)
				2. Life membership for Indian Nuclear Society (INS)
				3. Life member in Indian crystallographic association (ICA)

**National Conference/ International Conference / Papers Presented:**

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| **Sl.no** | **Title of the Paper** | **Dates** | **Conference where presented** |
| 1. | 1-Formyl-r -2,c-6-bis(4-methoxyphenyl)-t -3-methylpiperidin-4-one | 10th&11th March 2010 | Alagappa University, Karaikudi. |
| 2. | 2-(4-Fluorophenyl)-4,5-dimethyl-1-(4-methylphenyl)-1h-imidazole | 29th July 2011 | Periyar Maniammai University, Thanjavur |
| 3. | Poster presentation – “ X-Ray Crystallography” | 9th sep 2010 | Periyar Maniammai University, Thanjavur |
| 4. | “**X – fÂ® goféaš X® MŒÎ”** | 01.10.11 & 02.10.11 | Periyar Maniammai University, Thanjavur |
| 5. | x- ray crystal and molecular structure of r-2,c-6-bis(4-methoxyphenyl)-c-3,t-3-dimethylpiperidin-4-one | 8 to 10 october 2012 | Madras university Chennai |
| 6. | Growth and Characterization Studies on second ,third order non- linear optical :l-argininium p-tolene sulphate monohydrade crystal | Feb 2019 | International conferencePMIST |

**Participation in conference / workshops / seminars/ symposia / courses.**

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| **Sl.no** | **Title** | **Date** |
|  | Recent trends in Materials Science | 18th March 2009 |
|  | Teachers Development Programme on Testing and Evauation | 3rd to 6th March 2009 |
|  | Two day workshop on “Multimedia” | 25th -26th June 2009 |
|  | Educators Day 2009 the annual technical forum for faculty and research scholars. | 6th Dec 2009 |
|  |  Two weeks Staff Development Programme On “Role of cheminformatics in Drug Designing and Drug Discovery”. | 26th April to 7th May 2010. |
|  | Two weeks ISTE worshop on “Effective teaching / learning of Computer Programming”. | 28th June to 10th July 2010 |
|  | Instructional Design &Delivery System | 28th to 30th Oct 2010 |
|  | World Atheist Conference  | 7th to 9th Jan 2011 |
|  | One day workshop on SIX-SIGMA Yellow Belt Certification | 12th March 2011 |
|  | 19th National Scientific Tamil Conference  | 1.10.2011 to 2.10.2011 |
|  | Research Thesis/ Report Writing and e- Learning Content Preparation  | 3rd Nov to 4th Nov 2011 |
|  | Applications of MATLAB Software in Mathematical Field | 25th February 2012 |
|  | One day workshop on Radiochemistry | Apr. 28, 2012 |
|  | 3 days workshop on functional English for engineering teachers. | 23rd to 25th august 2012 |
|  | National seminar on crystallography | 8 to 10 october 2012 |
|  | 2 days ISTE workshop on Akash for Education | 10th& 11th November,2012 |
|  | National science day and Second scientific Tamil conference | 28.2.2013 |
|  | Two weeks ISTE workshop on Database Management System. | 21st to 31st May 2013 |
|  | one day workshop on LATEX software training programme  | 27th july 2013 |
|  |  Two weeks ISTE workshop in the title “ Engineering Mechanics”  | Nov 26th to 6th Dec 2013. |
|  | Three days conference at 6th Bangalore India nano conference  | Dec 4-6 2013. |
|  | ISTE Faculty convention,NEC Kovil patti | Nov 7th& 8th2014 |
|  | FDP on How to handle Adult | October 2014 |
|  | Atomic energy for building a better future & exhibition on BARC technologies | Feb. 14, 2015 |
|  | Outcome Based Education Workshop  | * 2.1.15,
* 4.5.2015 and 5.5.2015
* 14.05.2015 to 16.05.2015
 |
|  | Two weeks workshop on environment studies  | 2.6.15 to 12.6.15 |
|  | Two week ISTE short term training programme (STTP) on Engineering Physics  | 08th Dec to 18th December 2015 |
|  | One week refresher course on Instrumental method of Analysis | 17th may to 22nd May 2016 |
|  | Web of Science Advanced Series | October 7, 2019 |

**Special Lectures delivered:**

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| **S.No** | **Topic delivered** | **Organiser &Venue** | **Date** |
| 1. | e-content preparation | B. Ed ,PMU | Augustmonth, 2014 |
| 2. | Nobel Prize 2014 inPhysics | Department of Physics&ChemistryValluvar Hall | October18, 2014 |
| 3. | Journal publications | Faculty development programme , PMU | Dec 23, 2014 |
| 4. | Role of Youth inResearch | Kundhavai Naachiyar Govt. college, Thanjavur | Feb.23, 2015 |

**Research Laboratory / Industry visited** :

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| **SNO** | **Organization** | **Purpose** | **Duration** |
| 1.  | IISC , Bangalore | Visit to shock wave laboratory & Aerospace division | 2days ,2012 |
| 2. | ISRO, Trivandrum | RESPOND project discussion | 2 days ,2013 |
| 3. | IGCAR Kalpakkam | Theme meeting of Plutonium | 2 days, 2013 |
| 4. | Kudankulam | Nuclear plant visit | 1 day , 2014 |
| 5. | Madras university  | Training on Molecular docking studies  | 5 days Aug 2015. |