



Dr. Mahendra M., Ph.D., UGC Raman Fellow

Curriculum Vitae

Personal Information

Name : Mahendra M
Official Address : Associate Professor, Department of Studies in Physics,
Manasagangotri, University of Mysore, Mysuru, Karnataka,
570 006 INDIA.
Telephone : +91-821-2419603 (office)
+91-9964330328 (Mob.)
E-mail : mahendra@physics.uni-mysore.ac.in
mahendrashiri@gmail.com

Academic Profile

Bachelor of Science (1997) - University of Mysore, Mysuru, India.
Master of Science in Physics (1999) - University of Mysore, Mysuru, India.
PG Diploma in Software Development (2002) - University of Mysore, Mysuru, India.
Ph.D. in Physics (2005) - University of Mysore, Mysuru, India

Work Experience Details

Position	Institute	Duration
Associate Professor	DoS in Physics, University of Mysore, Manasagangotri	2020 to till date
Assistant Professor	DoS in Physics, University of Mysore, Manasagangotri	2007 to 2020
UGC Raman Post- Doctoral Fellow	Department of Cellular Biology and Pharmacology, Herbert Wertheim College of Medicine, Florida International University, Miami, USA	2014 to 2015
Post-Doctoral Research Associate	Biology Department, Brookhaven National Laboratory, Upton, New York, USA	2005 to 2007
CSIR Senior Research Fellow	DoS in Physics, University of Mysore, Manasagangotri	2004 to 2005
Ph.D. Research Scholar	DoS in Physics, University of Mysore, Manasagangotri	2000 to 2004
Research Assistant	JNCASR, Theoretical Sciences Unit, Bangalore	2000

Academic Affiliations/Awards

- **CSIR Senior Research Fellow Award**, Government of India (2004)
- **Post-Doctoral Fellow**, Brookhaven National Laboratory , Upton, NY, USA (2005-07)
- **UGC Raman Post-Doctoral Fellow**, Florida International University, Miami, FL, USA (2014-2015)
- **Life member**, Indian Crystallographic Association
- **Life member**, Indian Science Congress Association
- **Member**, American Crystallographic Association
- **Member**, New York Structural Genomics Consortium (NYSGXRC)
- **Member**, International Structural Genomics Organization (ISGO)

Research Projects:

Sl. No.	Title of the project	Principal/Co-Investigator	Funding Agency	Amount	Year (From-To)
1.	Structural studies of storage protein from the tuber of <i>amorphophalluspaeoniifolius</i> (Letter No. F. No. 41-920/2012(SR), Dated: 25-07-2012)	Principal Investigator	UGC, New Delhi	13,23,800 /- Lakhs	2012-2015
2	Molecular Docking and Crystallographic studies of Aminoglycoside N-acetyl transferases	Principal Investigator	Start Up Grant, University of Mysore	1 Lakh	2009-2011
3	Synthesis, growth and characterization of Chalcone based nonlinear optical materials	Principal Investigator	Minor Research Project, University of Mysore	75,000/-	2018-2019

Ph. D Candidates Currently Working/Finished:

Sl. No	Name of candidate	Subject	Thesis work	Status
1.	Mr. Chandra	Physics	Structure and Molecular Docking Studies of Some Biologically Important Compounds	Completed
2.	Mr. Nasseem Ahamad muhsen el-khatatneh	Physics	Crystal and Molecular Structure Studies of Some Medicinally Heterocyclic Compounds.	Completed

3.	Ms. Vishalakshi G. J	Biophysics	Exploring the Toxic Effects of Selected Phenolics on Platelets and Erythrocytes	Completed
4	Mr. Hussien Ahmed Hussien Khamees	Physics	Structural analysis and DFT studies of some biologically important compounds	Completed
5.	Mr. Ananda S	Physics	Studies on the Growth and Characterization of Some Nonlinear Optical Materials	Pursuing
6.	Ms. Bhavya N.R	Physics	Computational and Experimental Investigations on Some Fluorescent Materials	Pursuing
7.	Mr. Omantheswara N	Physics	Synthesis and Characterization of some Therapeutically important Compounds	Pursuing
8.	Mr. Keerthikumara V	Physics	Synthesis and Characterization of Nonlinear Optical Materials	Pursuing
9.	Mr. Keshav Kumar H	Physics	Computational and Experimental Investigations on Some Biosensors	Pursuing

Protein Structures Repository:

- Crystal structure of the human phosphatase (DUSP9). **PDB CODE:2HXP**
- Crystal structure of Hemolysin binding component from *Bacillus cereus*. **PDB CODE: 2NRJ**
- Crystal structure of a putative HTH-type transcriptional regulator ytcD. **PDB CODE: 2HZZ**
- Crystal structure of hypothetical protein TM1727 from *Thermatogammaritima*. **PDB CODE: 2I76**
- Crystal structure of YokD protein from *Bacillus subtilis*. **PDB CODE: 2NYG**
- Crystal structure of T110839 protein from *Synechococcus elongatus*. **PDB CODE: 2PLG**
- Crystal structure of CDP-diacylglycerolpyrophosphatase. **PDB CODE: 2POF**
- Crystal structure of mandelate racemase/muconate lactonizing enzyme-like protein from *Rubrobacter xylophilus* DSM 9941. **PDB CODE: 2QQ6**
- Crystal structure of the Mn(II)-bound glyoxalase from *Novosphingobium aromaticivorans*. **PDB CODE:3B59**
- Crystal structure of an uncharacterized protein from *Listeria monocytogenes*, trigonal form. **PDB CODE:3BQS.**

- Crystal structure of a protein of unknown function from *Listeria monocytogenes*, tetragonal form. **PDB CODE:3BQT**
- Crystal structure of a protein of unknown function from *Listeria monocytogenes*, triclinic form. **PDB CODE:3BQS**
- Crystal structure of a putative lactoylglutathionelyase from *Bdellovibriobacteriovorus*. **PDB CODE:3G12**

Crystal Structure of the complex formed between group II phospholipase A2 and a plant alkaloid ajmaline at 2.0 Å resolution. **PDB CODE: 1ZR8**

PUBLICATIONS

2021

1. Dithiane Based Boronic Acid as a Carbohydrate Sensor in an Aqueous Solution at pH 7.5: Theoretical and Experimental Approach: Bhavya N.R. and Mahendra M. *Journal of Fluorescence*, (2021), <https://doi.org/10.1007/s10895-021-02791-4>
2. Synthesis, Molecular Structure, DFT Studies, *In silico* Docking and Molecular Dynamics Simulations of 2, 6 dimethoxychalcone Derivatives as BRD4 Inhibitors: Hussien A. K., Mahendra M., Ananda S., Sangappa Y., Fares H. Al-Ostoot and Nadeem Abad. *Journal of Molecular Structure*, (2021), 1245, 131032
3. Synthesis, crystal structure, DFT calculations, Hirshfeld surface analysis, energy frameworks, molecular dynamics and docking studies of novel isoxazolequinoxaline derivative (IZQ) as anti-cancer drug: Nadeem A., Hamdi H. S., Fares H. Al-Ostoot, Hussien A. K., Sultan A. Al-horaibi, Shaukath A. K., Mahendra M., Mohamed El H., Joel T. M., El Mokhtar E. and Youssef R. *Journal of Molecular Structure*, (2021), 1232, 130004
4. Structural, thermal, dielectric, nonlinear optical properties and DFT investigations of a novel material 2-(6-chloropyridin-3-yl)-N'-(2, 3-dihydro-1, 4-benzodioxin-6-ylmethylidene) acetohydrazide for optoelectronic applications: Ananda S., Hussien A. K., Mahendra M., Kumara C., Jagadeesh Prasad D., Tejaswi A. H. and Vinitha G. *Journal of Materials Science: Materials in Electronics*, (2021), 32, 1-26
5. Design, synthesis, docking, Hirshfeld surface analysis and DFT calculations of 2-methylxanthen-9-with the FtsZ protein from *Staphylococcus aureus*: Ranganatha V. L., Mallikarjunaswamy C., Jagadeep Chandra S., Ramith R., Prithvi S. S., Naveen Kumar,

Sowmya B. P., Hussien A. K., Mahendra M. and Shaukath Ara K. *Bioinformation*, (2021), 17 (3), 393

2020

6. Pyridine based boronic acid carbohydrate sensor: DFT and spectroscopic investigations: Bhavya N. R., Ananda S., Khamees H. A. and Mahendra M. *AIP Conference Proceedings*, (2020), 2265 (1), 030360
7. Growth, crystal structure, Hirshfeld surface analysis, DFT and nonlinear optical studies of bis (4-methoxybenzylammonium) tetrachloridocadmate (II): Ananda S, Khamees H. A., Bhavya N. R. and Mahendra M. *AIP Conference Proceedings*, (2020), 2265 (1), 030408
8. Facile fabrication of silk fibroin microparticles: their characterization and potential adsorption study: Parushuram N., Ranjana R., Narayana B., Mahendra M. and Sangappa Y. *Journal of Dispersion Science and Technology*, (2020), 1-19.
9. Structural, Quantum Chemical and Spectroscopic Investigations on Photophysical Properties of Fluorescent Saccharide Sensor: Theoretical and Experimental Studies: Hussien A. Khamees, Bhavya N. R, Mahendra M, Jeyaseelan Sebastian, Doreswamy B. Haruvegowda and Shamantha Kumar. *ChemistrySelect*, (2020), 5, 5227-5238.
10. Fabrication and characterization of conductive silk fibroin-gold nanocomposite films: Ranjana R., Parushuram N., Harisha K. S., Asha S., Narayana B., Mahendra M., Sangappa Y. *Journal of Materials Science: Materials in Electronics*, (2020), 31(1), 249-264
11. Effect of o-difluoro and p-methyl substituents on the structure, optical properties and anti-inflammatory activity of phenoxy thiazole acetamide derivatives: Theoretical and experimental studies: Hussien Ahmed Khamees, Yasser Hussein Eissa Mohammed, Ananda S, Fares Hezam Al-Ostoot, Sangappa Y, Saad Alghamdi, Shaukath Ara Khanum, Mahendra M. *Journal of Molecular Structure*, (2020), 1199, 127024.

2019

12. Crystal structure, DFT calculation, Hirshfeld surface analysis and energy framework study of 6-bromo-2-(4-bromo-phen-yl)imidazo[1,2-a]pyridine: Hussien A. Khamees, Kumara C., Nasseem A. El-khatatneh, Ananda S., Kwong H. Chong, Jagadeesh Prasad D., and Mahendra Madegowda. *Acta Cryst.*, (2019), E75, 1620-1626.

13. Synthesis, crystal structure and studies of physical parameters of novel compound N-(2,6-dichlorophenyl)-4-(naphthalen-2-yl)-1,3-thiazol-2-amine: Gayathri B.H., Ravindra R.K., Jagadeesh Prasad D., Bhavya N.R., Lokanath N.K., Mahendra M., Laxmana K., Karegoudar Prakash. *Chemical Data Collections*, (2019), 24, 100286
14. Computational and spectroscopic investigations on boronic acid based fluorescent carbohydrate sensor in aqueous solution at physiological pH 7.5: N.R. Bhavya, M. Mahendra, H. B. Doreswamy, Shamantha Kumar, Maryam Gilandoust and Nasseem Ahmad El-khatatneh. *Journal of Molecular Structure*, (2019), 1197, 305-319.
15. Molecular Structure, DFT, Vibrational Spectra with Fluorescence Effect, Hirshfeld Surface, Docking Simulation and Antioxidant Activity of Thiazole Derivative: Hussien A. Khamees, Yasser H. E. Mohammed, Ananda Swamynayaka, Fares H. Al-Ostoot, Yusuf Sert, Saad Alghamdi, Shaukath A. Khanum, and Mahendra Madegowda. *ChemistrySelect*, (2019), 4, 4544 –4558
16. Zinc chloride catalyzed multicomponent synthesis of pyrazolopyridocoumarin scaffolds: Shamala D., Shivashankar K., Chandra and Mahendra M. *Journal of Chemical Sciences*, (2019), 131(4), 29.
17. Molecular docking and vibrational spectroscopy studies of (E)-N'-hydroxy-1, 3-diphenyl-4, 5-dihydro-1H-pyrazole-5-carboximidamide: Sert, Yusuf, Halil Gökce, M. Mahendra, N. Srikantamurthy, and Çağrı Çırak. *Journal of Molecular Structure*, (2019). 1184, 79-91.

2018

18. Para-tertiary butyl catechol (PTBC), an industrial antioxidant induces human platelet apoptosis: Vishalakshi GJ, NaveenKumar SK, Hemshekhar M, Mahendra M, Kemparaju K, Girish KS. *Environmental Toxicology*. (2018), 34(3), 262-270
19. 5-(1-Aryl-3-(thiophen-2-yl)-1H-pyrazol-4-yl)-1H-tetrazoles: Synthesis, structural characterization, Hirshfeld analysis, antiinflammatory and anti-bacterial studies: Mahadev N.K., Ravindra R.K., Jagadeesh Prasad D., Praveen K.B., Hussien Ahmed Khamees, Mahendra M., Shrinivas D. Joshi, Suneel Dodamani, Rasal V.P. and Sunil Jalalpure. *Journal of Molecular Structure*, (2018), 1160, 63–72.

20. Synthesis, Antimicrobial, Antioxidant and Molecular Docking Study of Some Novel Bis-1, 2, 4-Triazolo[3,4-B]-1,3,4-Thiadiazoles: Asma, Balakrishna Kalluraya, Manju N., Chandra, Mahendra M. and Revanasiddappa B.C. *Journal Of Medicinal Chemistry And Drug Design*, (2018), 1
21. Synthesis, crystal structure, spectroscopic characterization, docking simulation and density functional studies of 1-(3,4-dimethoxyphenyl) -3-(4-fluorophenyl)-propan-1-one: Hussien Ahmed Khamees, Mahima Jyothi, Shaukath Ara Khanum and Mahendra M. *Journal of Molecular Structure*, (2018), 1161, 199–217
22. Synthesis, Photophysical and Computational Study of Novel Coumarin-based Organic Dyes: Kumbar MN, Madivalagouda SS, Sannaikar MS, Shaikh SK, Kamble AA, Wari MN, Inamdar SR, Qiao Q, Bhavya NR, Mahendra M, Dasappa JP, Kamble RR. *Photochemistry and photobiology*, (2018), 94(2):261-76.

2017

23. Synthesis, Characterization and Molecular Docking of Novel Quinoline and Pyridine Derivatives: Saleh S., Al-Timari U., Al-Fahdawi A., El-Khatatneh N. and Mahendra M. *Oriental Journal of Chemistry*, (2017), 33(6), 2713-2719.
24. Synthesis, single crystal X-ray, Hirshfeld surface analysis and characterization of novel 4-(2, 4-dichlorophenyl)-N-(2, 6-dichlorophenyl)-1, 3-thiazol-2-amine: Gayathri, B. H., Dasappa, J. P., Bhavya, N. R., & Mahendra, M. *Journal of Molecular Structure*, (2017), 1146, 490-498.
25. Synthesis, Single Crystal X-ray and Hirshfeld Surface Analysis of (2-(methylthio)thiophen-3-yl)(thiophen-2-yl) methanone: El-khatatneh N., Kumara P., Khamees H., Sadashiva M. P., Jeyaseelan S. and Mahendra M. *Der Pharma Chemica*, (2017), 9(13), 32-39.
26. 5-[(Benzo [d][1, 3] dioxol-5-yl) methyl]-3-[4-(pyridin-2-yl) phenyl]-4, 5 dihydroisoxazole: El-Khatatneh, N., Vinayaka, A. C., Sadashiva, M. P., Jeyaseelan, S., and Mahendra M. *IUCrData*, (2017), 2(2), x170278.
27. 2-(2-Chlorobenzoyl)-1-(3, 4-dimethoxyphenyl)-3-iodoquinolin-4 (1H)-one: Kumar, S., Vinayaka, A. C., Mahendra, M., Sadashiva, M. P., & Doreswamy, B. H. *IUCrData*, (2017), 2(2), x170182
28. 2-(4-Methylphenyl)-2-oxoethyl 3,4-dimethoxybenzoate: Shamantha Kumar, Chandra, B. M. Rajesh, M. Mahendra and B. H. Doreswamy, *IUCrData*, (2017), 2, x170183

29. 6-tert-Butyl-4-[[4-hydroxymethyl-2H-1,2,3-triazol-2-yl)methyl]-2H-chromen-2-one.
Corrigendum: N El-Khatatneh, D Shamala, K Shivashankar, M Mahendra, *IUCrData*, (2017). 2(1), x170053
30. 4-[[4-Hydroxymethyl-2H-1,2,3-triazol-2-yl)methyl]-6,8-dimethyl-2H-chromen-2-one.
Corrigendum: N El-Khatatneh, D Shamala, K Shivashankar, M Mahendra, *IUCrData*, (2017). 2(1), x170052
31. (6-Fluoro-2-oxo-2H-chromen-4-yl)methyl diethylcarbamdithioate: N El-Khatatneh, BM Rajesh, S Kumar, BH Doreswamy, M Mahendra, *IUCrData*, (2017). 2(1), x162069
32. 4-[[4-Hydroxymethyl-2H-1, 2, 3-triazol-2-yl) methyl]-6-isopropyl-2H-chromen-2-one: El-Khatatneh, N., Shamala, D., Shivashankar, K., & Mahendra M., *IUCrData*, (2016), 1(12), x161989
33. 6-tert-Butyl-4-[[4-hydroxymethyl-2H-1, 2, 3-triazol-2-yl) methyl]-2H-chromen-2-one: El-Khatatneh, N., D. Shamala, K. Shivashankar, and M. Mahendra, *IUCrData*, (2016), 1(10), x161618

2016

34. 4-[[4-Hydroxymethyl-2H-1,2,3-triazol-2-yl)methyl]-6,8-dimethyl-2H-chromen-2-one: El-Khatatneh, N., Shamala D., Shivashankar K., & Mahendra M., *IUCrData*, (2016), 1(10), x161644
35. Methyl 2-(benzoyloxy) benzoate: S. Kumar, Chandra, C. S. Dileep, M. Mahendra, B. H. Doreswamy, *IUCrData*, (2016), 1(6), x160867.
36. AS3MT inhibitors: BP Rosen, H Dong, C Packianathan, M Madegowda, Arsenic Research and Global Sustainability: *Proceedings of the Sixth International Congress on Arsenic in the Environment* (As2016), June 19-23, 2016, pp 401-402, Stockholm, Sweden.
37. FeCl₃-Catalyzed Three-Component One-Pot Synthesis of Novel 4-[(Benzo [d] thiazol-2-ylamino)(phenyl) methyl]-3-hydroxy-9H-xanthen-9-ones: Cherkadu Vandana, Kalavagunta Praveen Kumar, Ningegowda Mallesha, Shivananju Nanjunda Swamy, Madegowda Mahendra, Babu Shubha Priya, *Synlett*. (2016), 27(7), 1116-1120.

38. Synthesis of N1 and N2 coumarin substituted 1,2,3-triazole isomers via click chemistry approach: Devadas Shamala, Kalegowda Shivashankar, Chandra, Madegowda Mahendra, *Synth Comm.*, (2016), 46(5), 434-441.
39. *Methyl 2-(benzoyloxy) benzoate*: S. Kumar, Chandra, C. S. Dileep, M. Mahendra, B. H. Doreswamy, *IUCrData*, (2016), 1(6), x160867.
40. *5-[[1-(2, 4-Dichlorophenyl)-1H-1, 2, 3-triazol-4-yl] methyl]-5H-dibenz [b, f] azepine*: K. S. Vinay Kumar, Chandra, B. M. Rajesh, M. Mahendra and M. P. Sadashiva,, *IUCrData*, (2016), 1(2), x160221.
41. *1-[(4-Methoxyphenyl) sulfonyl]-1H-indole-3-carbaldehyde*: E. A. Jithesh Babu, K. S. Vinay Kumar, Chandra, M. P. Sadashiva, M. Mahendra, *IUCrData*, (2016), 1(1), x160141.
42. *(7, 8-Dimethyl-2-oxo-2H-chromen-4-yl) methyl morpholine-4-carbodithioate*: S. Kumar, Chandra, A. A. Hosamani, M. Mahendra, B. H. Doreswamy, *IUCrData*, (2016), 1(1), x160084.

2015

43. Identification of small molecule inhibitors of human As (III) S-adenosylmethionine methyltransferase (AS3MT): Dong, Hui, Mahendra Madegowda, Adel Nefzi, Richard A. Houghten, Marc A. Giulianotti, and Barry P. Rosen. *Chemical research in toxicology*, (2015), 28(12), 2419-2425.
44. ArsP: a methylarsenite efflux permease. Chen, Jian, Mahendra Madegowda, Hiranmoy Bhattacharjee, and Barry P. Rosen. *Molecular microbiology*, (2015), 98(4), 625-635.
45. A Nano-MgO and Ionic Liquid-Catalyzed 'Green' Synthesis Protocol for the Development of Adamantyl-Imidazolo-Thiadiazoles as Anti-Tuberculosis Agents Targeting Sterol 14 α -Demethylase (CYP51): Sebastian Anusha, Baburajeev CP, Chakrabhavi Dhananjaya Mohan, Jessin Mathai, Shobith Rangappa, Surender Mohan, Chandra, Shardul Paricharak, Lewis Mervin, Julian E. Fuchs, Mahendra M, Andreas Bender, Basappa, K. S. Rangappa, *PLoS One.*, (2015), 10(10), e0139798. doi: 10.1371.
46. Crystal structure of 10-((3-oxo-3H-benzo[f]chromen-1-yl) methyl)-2-(trifluoromethyl) -9a,10-dihydrobenzo[4,5]imidazo[1,2-a]pyrimidin-4(5aH)-one: Chandra, Shamantha Kumar, K. B. Puttaraju, K. Shivashankar and Mahendra M., *Acta Cryst.*, (2015), 71, o672-o673.
47. Synthesis and characterization of novel oxazines and demonstration that they specifically target cyclooxygenase 2: V. Srinivas, C. D. Mohan, C. P. Baburajeev, R. Shobith, Julian E. Fuchs, Alexey Yu. Sukhorukov, Chandra, Daniel J. Mason, K. S. Sharath Kumar, M. Mahendra, Andreas Bender, Basappa, K. S. Rangappa, *Bioorganic & Medicinal Chemistry Letters*, (2015), 25, 2931-2936.

48. Crystal structure of 4-azidomethyl-6-tert-butyl-2H-chromen-2-one: Nasseem El-Khatatneh, Chandra, D. Shamala, K. Shivashankar, Mukhokosi Emma Panzia and M. Mahendra, *Acta Cryst.*, (2015), E71, o218-o219.
49. Crystal structure of 2-(4-methylphenyl)-4H-1,3-benzothiazine: N. C. Sandhya, Chandra, G. P. Suresha, N. K. Lokanath and M. Mahendra, *ActaCryst.*, (2015), E71, o74.
50. FT-IR, Laser-Raman spectra and computational analysis of 5-Methyl-3-phenylisoxazole-4-carboxylic acid: Yusuf Sert, M. Mahendra, S. Keskinoglu, Chandra, N. Srikantamurthy, K. B. Umesha, C. Cirak, *SpectrochimicaActa Part A: Molecular and Biomolecular Spectroscopy*, (2015), 139, 145-155.

2014

51. Molecular docking of 1H-pyrazole derivatives to receptor tyrosine kinase and protein kinase for screening potential inhibitors: Chandra, Vishalakshi G. J., Doreswamy B. H., Srikantamurthy N., Umesha N., Kemparaju K & Mahendra M. *Bioinformation*, (2014), 10(7), 413-418.
52. Ethyl 5-oxo-4-phenyl-5,6-dihydro-4H-1,3,4-oxadiazine-2-carboxylate: K. Shubakara, Chandra, N. Srikantamurthy, M. Mahendra and K. B. Umesha, *ActaCryst.* (2014), E70, o661.
53. Molecular docking studies of benzimidazopyrimidine and coumarin substituted benzimidazopyrimidine derivatives: As potential human Aurora A kinase inhibitors: Chandra, Puttaraju K. B., Mahesh S. S., Shivashankar K., Lokanath N. K. & Mahendra M. *Bioinformation*, (2014), 10(5), 288-292.
54. One-Pot Tandem Synthesis of TetrasubstitutedPyrazoles via 1,3-dipolar Cycloaddition Between Aryl Hydrazones and Ethyl But-2-ynoate: Srikantamurthy Ni, Shridevi D., Chandra, Mahendra M, Shubakara K & Umesha K. B. *Synthetic Communications: An International Journal for Rapid Communication of Synthetic Organic Chemistry*, (2014), 44: 2222-2231.
55. Synthesis and crystal structure studies of ethyl 5-methyl-1, 3-diphenyl-1H-pyrazole-4-carboxylate: Chandra, N. Srikantamurthy, E. A. JitheshBabu, K. B. Umesha, and M. Mahendra. *AIP Conference Proceedings* 1591, 1197 (2014); doi: 10.1063/1.4872901.
56. Vibrational spectroscopy investigation using M06-2X and B3LYP methods analysis on the structure of 2-Trifluoromethyl-10H-benzo[4,5]-imidazo[1,2-a]pyrimidin-4-one: Yusuf Sert, M. Mahendra, Chandra, K. Shivashankar, K. B. Puttaraju, H. Doğan, ÇağrıÇirak,

FatihUcun, *SpectrochimicaActa Part A: Molecular and Biomolecular Spectroscopy*, (2014), 128, 109-118.

57. Synthesis and characterization of stable nitrenium ion complex: 1-hydroxy-3-methyl benzotriazoliumtrifluoromethane sulfonate: B. H. Doreswamy, Chandra, K. Mantelingu, M. A. Sridhar, Mahendra M., *Res. Chem. Intermed.*, (2014), 40, 2659-2665.

2013

58. N-Benzoyl-5-methyl-1,3-diphenyl-1Hpyrazole-4-carbohydrazide: Chandra, N. Srikantamurthy, Shamanth Kumar, B. H. Doreswamy, K. B. Umesha and Mahendra M., *ActaCryst.* (2013), E69, o1769.
59. 5-Methyl-1,3-diphenyl-N-(5-phenyl-1,3,4-thiadiazol-2-yl)-1H-pyrazole-4-carboxamide: Chandra, K. Mahesh, N. Srikantamurthy, K. B. Umesha, K. Palani and M. Mahendra, *ActaCryst.* (2013), E69, o1736.
60. Trifluoromethyl-10H-benzo[4,5]imidazo[1,2-a]pyrimidin-4-one: Chandra, K. B. Puttaraju, K. Shivashankar, E. A. JitheshBabu and M. Mahendra, *ActaCryst.* (2013), E69, o1536.
61. Microwave assisted synthesis of dihydrobenzo[4,5]imidazo[1,2-a]pyrimidin-4-ones; synthesis, *in vitro* antimicrobial and anticancer activities of novel coumarin substituted dihydrobenzo[4,5]imidazo[1,2-a]pyrimidin-4-ones. K. B. Puttaraju, K. Shivashankar, Chandra, M. Mahendra, V. P. Rasal, P. N. Venkatavivek, K. Rai, M. B. Chanu, *European Journal of Medicinal Chemistry*, (2013), 69, 316-322.
62. Ethyl 1,4-bis(4-chlorophenyl)-2-methyl-1H-pyrrole-3-carboxylate: K. N. Nandeesh, Chandra, K. Palani, M. Mahendra and K. Mantelingu, *ActaCryst.* (2013), E69, o1269.
63. 2-(benzo[d][1,3]dioxol-5-yl)-3-phenylquinazolin-4(3H)-one: Chandra, G. M. Raghavendra, S. Jeyaseelan, K. Mantelingu and M. Mahendra, *ActaCryst.* (2013), E69, o1113.
64. A simple and efficient synthesis of substituted pyrazoles: Doddamani Shridevi Doddaramappa, Chandra, M. Mahendra and K. M. Lokanatha Rai, *Chemistry of Heterocyclic Compounds.* (2013), 49(5), 798-703.
65. Ethyl 5-methyl-3-phenylisoxazole-4-carboxylate: Chandra, K. Raghu, S. Jeyaseelan, K. B. Umesha and M. Mahendra, *ActaCryst.* (2013), E69, o987.
66. 5-methyl-3-phenylisoxazole-4-carboxylic acid: Chandra, N. Srikantamurthy, G. J, Vishalakshi, S. Jeyaseelan, K. B. Umesha and M. Mahendra, *ActaCryst.* (2013). E69, o897.

67. Synthesis and characterization of stable nitrenium ion complex: 1-hydroxy-3-methyl benzotriazoliumtrifluoromethane sulfonate: B. H. Doreswamy, Chandra, K. Mantelingu, M. A. Sridhar, M. Mahendra, *Res. Chem. Intermed.*, (2013), 40, 2659-2665

68. 3-(4-Methoxyphenyl)-5-methylisoxazole-4-carboxylic acid: Chandra, K. Raghu, N. Srikantamurthy, K. B. Umesha, K. Palani and M. Mahendra, *ActaCryst.* (2013), E69, o388.

2012

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120. Synthesis and crystal structure of 1-methyl-3-(4-nitrophenyl)-1,2,3 triazolium perchlorate: Doreswamy B.H., Mahendra M., Sridhar M.A., Shashidhara Prasad J., Mantelingu K., Basappa S. and Rangappa K.S., *Mol. Cryst. Liq. Cryst.*, (2003), 403, 67.
121. Structural studies on praseodymium malonate hydrate: Doreswamy B.H., Mahendra M., Sridhar M.A., Shashidhara Prasad J., Varughese P.A., Saban K.V. and George Varghese, *J. Mol. Str.*, (2003), 659, 81.

Meetings/Conferences/Workshops Attended

1. Presented paper entitle "Experimental and Theoretical Studies of Organic Nonlinear Optical Material: Acetohy-drazide Derivative" at the four days DAE-BRNS National Laser Symposium (NLS-28) Conference will be held at Vellore Institute of Technology, Chennai, Tamilnadu, from 08th January 2020 to 11th January 2020.
2. Presented paper entitle "Pyridine based boronic acidas carbohydrate sensor: DFT and spectroscopic investigations" at the five days 64th DAE Solid State Physics Symposium will be held at Indian Institute of Technology Jodhpur, Rajasthan from 16th December 2019 to 24th December 2019
3. Presented a paper entitled "Synthesis, Crystal structure, Hirshfeld surface analysis, DFT and Nonlinear optical studies: Acetohydrazide Derivative" at the "Current Application in Material Science" held at SJB Institute of Technology Kengeri, Bengaluru on May 4th, 2019.
4. Presented a paper entitled "Synthesis, Crystal structure, Hirshfeld surface analysis, DFT and Nonlinear optical studies of 2-(6-chloropyridin-3-yl)-N'-(2,3-dihydro-1,4-benzodioxin-6-ylmethylidene)acetohydrazide" at the "Advanced Functional Materials for Energy, Environment and Health Care (AFMEEHC)" held at Vijnan Bhavan, University of Mysore, Mysuru on March 18th to 20th, 2019.
5. Participated in the three day lecture workshop on "Quantum Statistics-Theory & Experiments" organised by the Department of Physics, St. Philomena's College (Autonomous), Mysuru, in association with science Academies of India from February 15th to 17th 2019.
6. Participated in the three day refresher course organised by Committee for the Development of Science in Schools, in Vijnan Bhavan, University of Mysore, Mysuru from September 18th to 20th 2019.

7. Presented a paper entitled "Synthesis, Crystal structure, Hirshfeld surface analysis, DFT and Nonlinear optical studies of Bis(4-methylbenzylammonium) Tetrachloridocuprate(II)" at the "46th National Seminar on Crystallography 2018" held at NIMHANS, Bengaluru on June 27th to 29th, 2018.
8. Participated in the three day lecture workshop on "Quantum Information and Computation" organised by the Department of Physics, St. Philomena's College (Autonomous), Mysuru, in association with science Academies of India from August 18th to 20th 2018.
9. Participated in the "Twenty-ninth Mid-Year Meeting of the Indian Academy of Science" held in Infosys Training Centre, Mysuru from June 29th to 30th 2018.
10. Presented a paper entitled "Crystal Structure and DFT Studies on Bio-sensing Material: 2-ethoxy-4-fluorophenylboronic acid" at the "Current application in Material Science" held at SJB Institute of Technology Kengeri, Bengaluru on May 9th, 2018.
11. Participated in the "Special Lecture Series in Environmental science", sponsored by University with Potential for Excellence held from March 16th to 19th 2018 at the Department of studies in Environmental Science, Manasagangotri, Mysuru-06
12. Participated in the three day lecture workshop on "Frontiers in Astronomy" organised by the Department of Physics, St. Philomena's College (Autonomous), Mysuru, in association with science Academies of India from February 17th to 19th 2018.
13. Participated in the National Conference on "Geometric Function Theory and its Application" organized by University of Mysore (UPE) held at Department of Studies in Physics, Manasagangotri, Mysuru from January 29th to 30th 2018.
14. Presented a paper entitled "Synthesis, Single Crystal X-ray and Computational studies of (4-chlorophenyl) (2-(methylthio) thiophen-3-yl) methanone" at the "Recent Advances in Materials Science and Biophysics (RAMSB)" held at Mangalore University, Mangaluru on January 23rd to 25th, 2018.
15. Participated in the "10th Annual Conference of Karnataka Science and Technology Academy 2018" jointly organized by Karnataka Science and Technology Academy and REVA University held during January 18th to 19th 2018.
16. Participated in the Eight Days National Training on "Application and Trouble Shooting of Scientific Equipment" organized by Institution of Excellence in association with UPE, University of Mysore, Vijnana Bhavana, Mysuru from December 01st to 08th 2017.

17. Presented a paper entitled "Crystal structure of N-(2, 6-dichlorobenzylidene)-3,5-dichlorobenzamine" at the "Recent Trends in Material Science and Environmental Issues" held at SJB Institute of Technology Kengeri, Bengaluru on May 10th, 2017.
18. Participated in the Science Academies 84th 16 day Refresher Course " In Experimental Physics" organized by the Department of Physics, St. Philomena's College (Autonomous), Mysuru from February 14th to march 1st 2017.
19. Participated as a delegate in the "XL Indian Social Science Congress" jointly organized by Indian Academy of Social Sciences and University of Mysore, held at DOS in Physics, University of Mysore, Mysuru from December 19th to 23rd 2016.
20. Participated in the "103rd Indian Science Congress" held at University of Mysore, Mysuru from January 3rd to 7th 2016.
21. Presented a paper entitled "Crystal structure of a putative NADP dependent oxidoreductase TM1727 from *Thermotoga maritima*" at the "5th Winter School Soft X-rays in Macromolecular Crystallography", University of Georgia, Athens, USA held on March 1st to 4th, 2015.
22. Participated as a delegate in the one-day seminar on "Radioactivity- Natural and Manmade", organized by Indian Nuclear Society, Mysore and Vidya Vikas Institute of Engineering and Technology at VVIET Campus, Mysore held on March 15th, 2014.
23. Presented a paper entitled "Synthesis and Structural Studies of Ethyl 2-methyl-4-phenyl-1-(4-(trifluoromethyl)benzyl)-1H-pyrrole-3-carboxylate" at the UGC sponsored two days National Seminar on "Material Science and Engineering (NSMSE)", held at JSS College of Arts, Commerce and Science, Mysore during March 21-22nd, 2014.
24. Presented a paper entitled "Synthesis and characterization of novel Ethyl 5-oxo-4-phenyl-5,6-dihydro-4H-1,3,4-oxadiazine-2-carboxylate" at the International Symposium on Chemical Biology- Drug Discovery Programme, held at University of Mysore, Mysore during January 9-10th, 2014.
25. Presented a paper entitled "Structure of conserved hypothetical protein TM1727 from *Thermatoga maritime*: a probable NADP dependent-dehydrogenase" at the International Symposium on Chemical Biology- Drug Discovery Programme, held at University of Myore, Mysore during January 9-10th, 2014.

26. Presented a paper entitled “ Synthesis and crystal structure studies of Ethyl 4-methyl-1, 3-diphenyl-1*H*- pyrazole-5-carboxylate” at the 58th DAE Solid State Physics Symposium, held at Thapar University, Patiala, Punjab during December 17-21, 2013.
27. Presented a paper entitled “Synthesis and crystal structure studies of Ethyl 5-methyl-1, 3-diphenyl-1*H*- pyrazole-4-carboxylate” at the 42nd National Seminar on Crystallography and International Workshop on Application of X-ray Diffraction for Drug Discovery, held at Jawaharlal Nehru University, New Delhi during November 21-23, 2013.
28. Presented a paper entitled “Hydrothermal synthesis, crystal structure and characterization of $\text{LiSrHP}_2\text{O}_7$ ” at the National seminar on Current Trends of Research in Precambrian Geology and Vision 2020, held at Department of Studies in Earth Science, University of Mysore, Manasagangotri, Mysore during March 20-21, 2013.
29. Participated as a delegate in the Four-day National workshop on “Basic techniques in molecular biology and bioinformatics”, organized by postgraduate department of Biotechnology, JSS College for Arts, Commerce and Science, Ooty road, Mysore, in association with association of Microbiologists of India (AMI) (Mysore chapter) and BIORAD, held from 15th to 18th March 2013.
30. Presented a paper entitled “Structure of putative aminoglycoside N-Acetyl transferase from *Bacillus subtilis*” at the International Conference on Biomolecular Forms and Functions, held at J. N. Tata Auditorium, Indian Institute of Science, Bangalore during January 8-11, 2013.
31. Presented a paper entitled “Growth and Characterization of a Semi-organic NLO Material: L-Serine Potassium Nitrate ” at the 24th National Seminar on Crystal Growth, held at Anna University, Chennai, India during December 20-22, 2012.
32. Participated as a delegate in the one-day technical seminar on “Nuclear Energy- Environment and Safety” (NEEDS-2012), Jointly organized by Indian Nuclear Society, Mysore and Department of Studies in Physics, University of Mysore on 3rd March 2012 at DOS in Physics, University of Mysore, Mysore.
33. Presented a paper entitled “Crystal structure studies of Diethyl-(6-chloro-2-carbazolyl)methyl malonate an intermediate in the synthesis of anti-inflammatory drug Carprofen” at the 40th International Seminar on Crystallography, held at Osmania University, Hyderabad, India during November 26-28, 2011.

34. Presented a paper entitled "Synthesis and Crystal Structure of stable nitrogen ion complex: 1-Hydroxy-3-methyl benzotriazoliumtrifluoromethane sulfonate" at the National Conference on "Recent trends in Material Chemistry and Engineering (RTMCE- 2011), held at Department of Chemistry, RNS Institute of Technology, Bangalore, India during September 29-30, 2011.
35. Participated 'UGC Sponsored Refresher Course in Physics, Batch -XVII' held from September 8th to 28th 2011, at Academic Staff College, University of Madras, Chennai.
36. Participated 'UGC Sponsored National Conference on Applications of Mathematics and Statistics' held at Yuvaraja's College, Mysore during March 25-26, 2011.
37. Presented a paper entitled "X-ray Structure of Aminoglycoside 3-n-acetyl transferase (YokD) from *Bacillus Subtilis*" at the International Symposium on Challenges in Drug Discovery Programme- 2011 (ISCDDP-2011) held at KSOU, Manasagangothri, Mysore, India during February 16-17, 2011.
38. Presented a paper entitled "Synthesis and Crystal structure of a novel antibacterial drug: 1,2-Bis(N-methylbenzimidazolyl)benzene" at the International Symposium on Challenges in Drug Discovery Programme- 2011 (ISCDDP-2011) held at KSOU, Manasagangothri, Mysore, India during February 16-17, 2011.
39. Presented a paper entitled " Structure and Docking studies of Aminoglycoside 3-N-acetyltransferase from *Bacillus subtilis*" at the 6th International Structural Biology and Functional Genomics Conference, Dec 6-8, 2010, National University of Singapore, Singapore.
40. Participated 'Science Academies' Lecture Workshop on some topics in "Biophysics" at Department of Studies in Physics, University of Mysore, Mysore, India, Sep 16-17, 2010.
41. Participated the State Inter University meeting of Vision Group on Science and Technology in Physics, Chemistry and Material Science subjects at Department of Studies in Physics, University of Mysore, Mysore, India, March 08-09, 2010.
42. Presented a paper entitled "Crystal structure of yokD protein from *Bacillus subtilis*" at the 8th Asia Pacific Bioinformatics Conference, Bangalore, India, Jan 18-21, 2010.

43. Participated UGC sponsored 84th Orientation course at Academic Staff College, University of Mysore, Mysore, Oct 7th to 3rd November 2009.
44. Presented a paper entitled "Crystal Structure of Dual Specificity Human Phosphatase DUSP9" at the 38th National Seminar on Crystallography, University of Mysore, Mysore, Feb 11-13, 2009.
45. Presented a paper entitled "Synthesis and X-ray Structure of 1,2-bis(N-methylbenzimidazolyl)Benzene" at the 38th National Seminar on Crystallography, University of Mysore, Mysore, Feb 11-13, 2009.
46. Presented a paper "Crystal structure of hypothetical protein TM1727 from *Thermatogamaritima*" at the American Crystallographic Association, Honalulu, Hawaii, USA, July 21-26, 2006.
47. Presented a paper entitled "Crystal Structure of Novel 2-butyl-4-chloro-1H-Imidazolyl-5-Carboxaldehyde", at the XXXIII National Seminar on Crystallography, National Chemical Laboratory, Pune, January 8-10, 2004.
48. Presented a paper entitled "Synthesis and X-ray Structure of 1,2-bis(N-methylbenzimidazolyl)benzene", at the XXXIII National Seminar on Crystallography, National Chemical Laboratory, Pune, January 8-10, 2004.
49. Presented a paper entitled "Crystal Structure of 1-methyl-3-(4-nitrophenyl)-1,2,3-triazolium perchlorate", at the XXXIII National Seminar on Crystallography, National Chemical Laboratory, Pune, January 8-10, 2004.
50. Presented a paper entitled "Hydrothermal Synthesis and Structure of New Condensed Hydrated Lithium Cobalt Pentaphosphate", at the DAE-Solid State Physics Symposium, Jiwaji University, Gwalior, India, December 26-30, 2003.
51. Presented a paper entitled "Structural studies of Samarium malonate hexahydrate", at the DAE-Solid State Physics Symposium, Jiwaji University, Gwalior, India, December 26-30, 2003.
52. Participated in Indo-German school on Synchrotron Radiation Sources and their Applications at Centre for Advanced Technology, Indore, India, November 11-22-2002.

53. Presented a paper entitled "Crystalline structural studies of solid electrolyte compounds like $M^+NiP_2O_7$ [$M^+=Na, Cs$]", at the XXXII National Seminar on Crystallography held at University of Jammu, Jammu Tawi, India, October 24–26, 2002.
54. Presented a paper entitled "Synthesis and structural characterization of solid electrolyte compound $CsCoP_2O_7$ ", at the XXXII National Seminar on Crystallography held at University of Jammu, Jammu Tawi, India, October 24–26, 2002.
55. Presented a paper entitled "Structure analysis of tetra thiourea copper(II) chloride complex", at the XXXII National Seminar on Crystallography held at University of Jammu, Jammu Tawi, India, October 24–26, 2002.
56. Participated in the International Conference on "Problems and Prospect of IT Professionals in the New Millenium" and National Seminar on "World Wide Web Education", University of Mysore, Mysore, January 13-16, 2002.
57. Presented a paper entitled "Crystal and Molecular structure studies of LignocainiumOctochloroBis (μ -Dichloro) Dibismathate(III)", at the DAE-Solid State Physics Symposium, Bhabha Atomic Research Centre, Mumbai, December 26-30, 2001.
58. Attended the meeting of International symposium on Crystallography and Bioinformatics in Structural Biology, at IISc and National centre for Biological Sciences, Bangalore, November 22-25, 2001.
59. Attended the IV meeting of Asian Crystallographic Association held at Indian Institute of Science. Bangalore, India, November 18-21, 2001.

Research lab facilities and ongoing research work plan

Crystallography and Computational Lab

➤ Research Supervisor: **Dr. Mahendra M**

➤ Research Scholars: Ananda S, Bhavya N.R and Hussien Ahmed Khamees

<u>Crystallography Lab Facilities</u>	<u>Computational Lab Facilities</u>	<u>Achievements</u>
<ul style="list-style-type: none">• Magnetic Stirrers• Electronic Weighing balance• UV Chamber• Refrigerator and Deep Freezer• Incubator• Dancing shaker, Vortex• Revolutionary High speed table top cooling centrifuge• pH meter	<ul style="list-style-type: none">• Gaussian09 Software• GaussView Software• High Performance Quad core Computer	<ul style="list-style-type: none">• Publications - 111• Abroad Visit – Dr. Mahendra M as Research Associate, BNL, NY, USA and Raman Fellow, Miami, USA• Best Poster Award – 2 (2018 and 2019)• Junior Research Fellows – 2 (CSIR-UGC and DST)• Foreign Scholar – 1 (Yemen National)• Ph.D. Awarded – 2

