BHOLANATH MANDAL, M. Sc., Ph.D.

Contact Information

Professor
Department of Chemistry
The University of Burdwan
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Sex/ Marital status: Male/ Married

Education

- Ph. D., The University of Burdwan, 2006
  (Thesis: GRAPH THEORETICAL STUDIES ON FULLERENES AND SOME SYSTEMS OF CHEMICAL INTEREST)
- NET (Joint CSIR-UGC), JRF (UGC), 1994
- GATE (Dept. of Education, Ministry of HRD, Govt. of India), 1994
- M. Sc. (Chemistry), The University of Burdwan, 1993
  (Field of Specialization: Physical Chemistry)
- B. Sc. (Honours in Chemistry), The University of Burdwan, 1991
  (College attended: Ramananda College, Bishnupur, Bankura-722 122, WB, India)

Teaching Experience

- Lecturer in Chemistry (WBES), A. B. N. Seal College, Cooch Behar, WB (July 01, 1998 – September 30, 1999)
- Lecturer in Physical Chemistry, Department of Chemistry, The University of Burdwan (October 01, 1999 – June 30, 2004)
- Senior Lecturer in Chemistry, Department of Chemistry, The University of Burdwan (July 01, 2004 – June 30, 2007)
- Reader in Chemistry, Department of Chemistry, The University of Burdwan (July 01, 2007 – June 30, 2010)
- Associate Professor of Chemistry, Department of Chemistry, The University of Burdwan (July 01, 2010 –January 09, 2017)
- Professor of Chemistry, Department of Chemistry, The University of Burdwan (January 10, 2017–)

Administrative Experience

- Head of the Department of Chemistry, of the University of Burdwan (September 01, 2014 to August 31, 2016)
- Chairman of Board of Post Graduate Studies in Chemistry of the University of Burdwan (September 01, 2014 to August 31, 2016)
- Chairman of Board of Under Graduate Studies in Chemistry of the University of Burdwan (September 01, 2014 to August 31, 2016)

Post Doctoral Experience

Worked as Post Doctoral Fellow at Texas A & M University @ Galveston, Texas -77553, USA for the period from October 01, 2010 to May 31, 2012 with Professor Douglas J. Klein

Research interests

Area of research interest is primarily theoretical that concerns the application of Graph Theory

- to study the eigenspectral properties of some molecular systems (starting from small to extended polymeric structures),
- to develop algorithms for calculation of Topological Indices (TIs) and their uses in QSAR and QSPR studies,
- to deal with problems involving reaction networks, etc.

Life Membership

- Indian Physical Society
- Indian Chemical Society
- Chemical Research Society of India

Research Scholars

Sl. No	Name	Title of Thesis	Part-time/ full-time	Awarded/ Submitted
1.	Piyali Ghosh	Studies on physicochemical properties of open and closed π-conjugated networks from graph theoretical point of view	Part-time	Awarded degree (Ph. D.) on September 28, 2015
2.	Somnath Karmakar	Study on some π-conjugated molecules and reaction networks in the light of graph theory	Part-time	Awarded degree (Ph. D.) on December 13, 2016
3.	Tapanendu Ghosh	Theoretical studies on topology related properties of some chemical structures	Part-time	Awarded degree (Ph. D.) on September 12, 2019
4.	Sukanya Mondal	Experimental and theoretical studies on some reaction networks	Full-time (01-08-2013 to 16-08-2016)/ Part-time	Working
5.	Swapnadeep Mondal		Full-time (CSIR Fellow)	Working

M. Phil. Guidance

Sl. No.	Student's Name	Title of the dissertation	Supervisor(s)	Degree awarded
1.	Biswajit Mandal	Effect of solvent polarity on the stability and CT transition energy of the naphthalene-p-chloranil complex	Jointly with Professor A. K. Mukherjee	Awarded (2010)

Research Project

Sl. No	Title of the project	Agency (Funding, Commissioning and/or Collaborating)	Period	Grant(s)/ Amount mobilized (so far) in Rupees	Whether Principal Investigator/ Coinvestigator or Consultant/Quality evaluator
1.	Study of aggregation carbon cluster in polar media	UGC (minor) Sanction No. RNI/472 (2000-2001)/89	2000-2001	14,500.00	PI

List of Publications

1. S. Mondal and **B. Mandal**, Sum of characteristic polynomial coefficients of cycloparaphenylene graphs as topological index, *Mol. Phys.*, 2019, (https://doi.org/10.1080/00268976.2019.1685693).
2. T. Ghosh, S. Mondal, S. Mondal and **B. Mandal**, Hückel Molecular Orbital Quantities of {X,Y}-Cyclacene Graphs Under Next-Nearest-Neighbour Approximations in Analytical Forms, *Z. Naturforsch*., 74 (6)a, 469-488 (2019).
3. S. Karmakar & **B. Mandal**, {*X*,*Y*}-Cyclacene Graphs with Next Nearest Neighbor Interactions, *Polycyl. Aromat. Comp*., **39**, 159-171 (2019).
4. S. Mondal and **B. Mandal**, Effect of surfactants on the B-Z reaction with ninhydrin as organic substrate, *Tenside Surf. Det.*, **55**, 196-202 (2018).
5. T. Ghosh, S. Mondal, S. Mondal and **B. Mandal**, Distance numbers and Hosoya indices of IPR fullerenes with formula $C_{10(n-2)}$ (n≥8) in analytical forms, *Chem. Phys. Lett.*, **701**, 72-80 (2018).
6. S. Mondal & **B. Mandal**, Procedures for Obtaining Characteristic Polynomials of the Kinetic Graphs of Reversible Reaction Networks, *Bull. Chem. Soc. Jpn.*, **91**, 700-709 (2018).
7. T. Ghosh, S. Mondal and **B. Mandal**, Matching polynomial coefficients and the Hosoya indices of poly (p-phenylene) graphs, *Mol. Phys.*, **116**, 361-377 (2018).
8. D. Ye, Y. Yang, **B. Mandal** & D. J. Klein, Graph invertibility and median eigenvalues, *Lin. Alg. Appl.*, **513**, 304-323 (2017).
9. T. Ghosh, S. Mondal, S. Karmakar and **B. Mandal**, Symmetry-adapted linear combinations for the eigenvalues and eigenvectors of reciprocal graphs, *Mol. Phys.*, **114**, 3307-3318 (2016)..
10. D. J. Klein and **B. Mandal**, Local Symmetries for Molecular Graphs, *MATCH Commun. Math. Comput. Chem.*, **74**, 247-258 (2015).
11. S. Karmakar, S. Mondal and **B. Mandal**, Eigensolutions of Cyclopolyacene Graphs, *Mol. Phys.* **113**, 719-726 (2015).
12. S. Karmakar and **B. Mandal**, Graph Theoretical Analysis on the Kinetic Rate Equations of Linear Chain and Cyclic Reaction Networks, *J. Phys. Chem. A*, **118**, 7672-7682 (2014).
13. P. Ghosh, S. Karmakar and **B. Mandal**, Matrix product forms for the characteristic polynomial coefficients of poly(*p*-phenylene) graphs, *J. Indian Chem. Soc.* - **91**, 2197-2210 (2014).

14. P. Ghosh, S. Karmakar and **B. Mandal**, Cardinalities of Poly(*p*-Phenylene) Graphs, *Mol. Phys.*, **112**, 2646-2653 (2014).
15. S. Karmakar and **B. Mandal**, Graph Theoretical Solutions for the Coupled Kinetic Rate Equations, *J. Phys. Chem. A*, **118**, 1155 – 1161 (2014).
16. P. Ghosh, D. J. Klein and **B. Mandal**, Analytical Eigenspectra of Alternant Edge Weighted Graphs of Linear Chains and Cycles: Some Applications, *Mol. Phys.*, **112**, 2093-2106 (2014).
17. P. Ghosh, S. Karmakar and **B. Mandal**, Eigensolutions of dodecahedron graphs, *Chem. Phys. Lett.*, **594**, 41 – 46 (2014).
18. **B. Mandal** and D. J. Klein, Characteristic polynomial followed by trigonometric identity for obtaining analytical eigenspectra of some weighted graphs of linear chains and cycles, *Bull. Chem. Soc. Jpn.*, **87**, 491-497 (2014).
19. P. Ghosh and B. **Mandal**, Formulas for the characteristic polynomial coefficients of the pendant graphs of linear chains, cycles and stars, *Mol. Phys.*, **112**, 1021 – 1029 (2014).
20. P. Ghosh, S. basu, S. Karmakar and **B. Mandal**, Schematic generation of characteristic polynomials and the Hosoya indices of mono- and di-substituted polymer graphs of linear chains and cycles, *J. Indian Chem. Soc.*, **91**, 503-515 (2014).
21. P. Ghosh, T. Ghosh and **B. Mandal**, Use of symmetry plane fragmentation and graph squaring technique to express eigenspectra for some vertex-weighted graphs of linear chains and cycles in analytical forms, *Mol. Phys.*, **109**, 267-277 (2011).
22. P. Ghosh and **B. Mandal**, Characteristic polynomials of alternant edge weighted linear chains with subsequent application to some linear poly (p-phenylene) graphs, *J. Math. Chem.*, **48,** 1069-1091 (2010).
23. S. Basu, P. Ghosh and **B. Mandal**, Algorithms to calculate the distance numbers and the Wiener indices of linear and cylindrical poly (*p*-phenylene) in terms of number of hexagonal rings, *Mol. Phys.*, **106**, 2507-2513 (2008).
24. A. S. Tiwary, **B. Mandal** and A. K. Mukherjee, Construction and studies of a new class of reciprocal trees: interknitting of the Pascal's triangle, *Mol. Phys.*, **106**, 1813-1821 (2008).
25. **B. Mandal**, Eigenspectral analysis of pendant vertex- and pendant edge-weighted graphs of linear chains, cycles, and stars, *Bull. Chem. Soc. Jpn.*, **81**, 956-965 (2008).
26. A. Ray and **B. Mandal**, Kinetic rate equation in integrated forms for single-step reactions involving different types of reactant, *Prog. React. Kinet. Mech.*, **33**, 267-281 (2008).
27. **B. Mandal**, Some important formulae using the concept of graphical tree, *Chem. Phys. Lett.*, **417**, 395-400 (2006).
28. **B. Mandal**, Use of symmetry plane and subsequent subtraction for obtaining eigenspectra of some complicated graphs in analytical forms, *J. Mol. Struct. (Theochem)*, **757**, 99-111 (2005).
29. **B. Mandal**, K. Datta, M. Banerjee and A. K. Mukherjee, Construction and utilisation of planar graphs of two series of IPR fullerenes through the use of threefold rotational symmetry, *Int. J. Quantum Chem.*, **105**, 201-208 (2005).

30. **B. Mandal**, M. Banerjee and A. K. Mukherjee, Wiener and Hosoya indices of reciprocal graphs, *Mol. Phys.*, **103**, 2665-2674 (2005).
31. **B. Mandal**, Graph theoretical procedure for obtaining analytical expressions of eigenspectra of linear chains and cycles with alternant vertex weights and same edge weight: Application to some complicated graphs, *Int. J. Quantum Chem.*, **103**, 140-148 (2005).
32. **B. Mandal**, M. Banerjee and A. K. Mukherjee, Construction of characteristic polynomial of reciprocal graphs from the number of pendant vertices, *Int. J. Quantum Chem.*, **101**, 119-126 (2005).
33. P. Pal, **B. Mandal**, K. Ray, A. K. Mukherjee and D. C. Mukherjee, Study of a reaction between 1,3-dinitrobenzene and acetophenone in presence of hydroxide ion, *J. Indian Chem. Soc.*, **81**, 1093-1096 (2004).
34. **B. Mandal**, M. Banerjee and A. K. Mukherjee, Construction of planar graphs for IPR fullerenes using 5- and 6-fold rotational symmetry: some eigenspectral analysis, *Phys. Chem. Chem. Phys.*, **6**, 2040-2043 (2004).
35. **B. Mandal**, M. Banerjee and A. K. Mukherjee, Cardinalities of reciprocal graphs, *Int. J. Quantum Chem.*, **99**, 119-126 (2004).
36. **B. Mandal**, K. Datta, A. K. Mukherjee and M. Banerjee, A Pascal's triangle-like approach for the determination of characteristic polynomial coefficients of reciprocal graphs, *Mol. Phys.*, **96**, 1609-1611 (1999).

Invited lectures in Symposia/Seminar/Conference/Workshop etc.

1. **B. Mandal**, Invited lecture on "Fractals in nano-regime" in the *Refresher Course in Chemistry* organized by **Human Resource Development Centre, The University of Burdwan** on July 01, 2019.
2. **B. Mandal**, Invited lecture on "C_{60} fullerene: an amazing carbon cluster" in the *Refresher Course in Chemistry* organized by **Human Resource Development Centre, The University of Burdwan** on September 25, 2019.
3. **B. Mandal**, Invited lecture on "Some mathematical aspects of interest in chemistry" in the Departmental Seminar organized by the **Department of Chemistry, K. C. College, Hetampur, Birbhum** on February 09, 2017.
4. **B. Mandal** , Invited lecture on "Graph theoretical eigensolutions of some molecular graphs" in the UGC Sponsored National on 'Chemistry today-nanoworld to Macroworld' organized by the **Department of Cheistry, Sonamukhi College, Sonamukhi, Bankura** in collaboration with the **Department of Chemistry, Indus Mahavidyalaya, Indus, Bankura** on December 22-23, 2016.
5. **B. Mandal**, "Graph Theory: A Tool to Solve Coupled Kinetic Rate Equations" in *Perspective in Teaching & Research in Physical Chemistry* organized by **Department of Physical Chemistry, Indian Association for the Cultivation of Science** on August 21-22, 2015.

6. **B. Mandal**, "Graph Theory: an indispensable tool to a Chemist" in *Modern Trends in Chemical Sciences* organized by **Bankura Christian College and the Chemical Society of the Chemistry Department of Bankura Christian College** on December 17, 2014.
7. **B. Mandal**, **"**A graph theoretic outlook on the structures and properties of carbon cages" in the *Refresher Course on nano-materials* organized by **Academic Staff College, The University of Burdwan** on July 10, 2013.
8. **B. Mandal**, "Symmetry and Graph Spectra" in *Math. and Science Seminar* organized by **GACD, Texas A & M University @Galveston, Texas, USA** on May 02, 2012.
9. **B. Mandal**, "Graph theory: Brief history and some aspects of interest in chemistry" in the *Refresher Course in Chemistry* organized by **Academic Staff College, The University of Burdwan** on September 10, 2010.

Seminar/Symposia/Workshop

1. Swapnadeep Mondal and **B. Mandal**, "Randić connectivity indices of the graphs of cyclacenes and cylindrical poly(p-phenylenes)" in the One Day National Level Seminar on *Design*, *Synthesis*, *Characterization*, *Reactivity*, *Theoretical Study and Applications of Different Advanced Functional Materials*, organized **Department of Chemistry of The University of Burdwan** on March 27, 2019
2. Swapnadeep Mondal, Tapanendu Ghosh and **B. Mandal**, "Bond Orders and Free Valence of Cyclacenes Graphs with Next Nearest Neighbour Interactions" in the National Seminar on *Design*, *Synthesis*, *Characterization*, *Reactivity*, *Theoretical Study and Applications of Different Advanced Functional Materials* organized **Department of Chemistry of The University of Burdwan** during December 21-23, 2017.
3. Tapanendu Ghosh and **B. Mandal**, "Wiener indices of a series of fullerene graphs ($C_{(n-2)10}$) in analytical forms" in the National Seminar on *Design*, *Synthesis*, *Characterization*, *Reactivity*, *Theoretical Study and Applications of Different Advanced Functional Materials* organized **Department of Chemistry of The University of Burdwan** during December 21-23, 2017.
4. S. Mondal and **B. Mandal**, "Investigation on the effect of anionic, cationic and neutral surfactants on the Belousov-Zhabatonsky (BZ) reaction" in three-Day National Level Seminar on *Design, Synthesis, Chemical and Biochemical Activities of Different Functional Molecules* organized by the **Department of Chemistry of The University of Burdwan** during February 04-06, 2016.
5. S. Karmakar and **B. Mandal**, "Eigensolutions of Cyclopolyacene Graphs with next nearest neighbor interactions" in three-Day National Level Seminar on *Design, Synthesis, Chemical and Biochemical Activities of Different Functional Molecules* organized by the **Department of Chemistry of The University of Burdwan** during February 04-06, 2016.

6. **B. Mandal**, "Symmetry Adapted Analytical Eigensolutions of Reciprocal Graphs" in the *National Symposium on Recent Advances in Chemistry and Industry (2015)* organized by the **Indian Chemical Society** on July 31 & August 01, 2015 at Meghnad Saha Bhavan, Kolkata.
7. S. Karmakar and **B. Mandal**, "Graph Theoretical Determination of the Concentrations of the Species Involved in Multistep Reactions" in *Advanced Spectroscopy, Theoretical Chemistry, Synthesis, Reactivity and Structural Evaluation* organized by the **Department of Chemistry of The University of Burdwan** on February 19-21, 2015.
8. S. Karmakar and **B. Mandal**, "Determination of Analytical Expression of the Eigenvalues of Dodecahedron Graph" in the *Modern Chemistry: An Interdisciplinary Science* organized by **Nistarini College, Purulia, WB** on January 19, 2015.
9. **B. Mandal**, "Utilization of symmetry plane fragmentation followed by simple subtraction for obtaining analytical graph eigenspectra" in *Acharya Prafulla Chandra Ray Memorial Symposium on Chemistry and Industry (2014)* organized by the **Indian Chemical Society** on August 01-02, 2014 at Meghnad Saha Bhavan, Kolkata.
10. S. Karmakar and **B. Mandal**, "Graph Theoretical Eigenvalues of Cyclopolyacene Graphs" in *Acharya Prafulla Chandra Ray Memorial Symposium on Chemistry and Industry (2014)* organized by the **Indian Chemical Society** on August 01-02, 2014 at Meghnad Saha Bhavan, Kolkata.
11. S. Karmakar and **B. Mandal**, "Determination of Total π-Electron Energy & HOMO-LUMO Gap in Cyclopolyacene Molecule: A Graph Theoretical Approach" in *Recent Progress in Chemistry-2014* organized **by Sidho-Kanho-Birsha University, Purulia, WB** on August 13, 2014.
12. **B. Mandal**, "Characteristic polynomial coefficients of the pendant graphs of linear chains with varying number of pendant vertices" in *Acharya Prafulla Chandra Ray Memorial Symposium on Chemistry and Industry (2013)* organized by the **Indian Chemical Society** on August 02-03, 2013 at Meghnad Saha Bhavan, Kolkata.
13. **B. Mandal**, Characteristic polynomial of linear poly (p-phenylene) (PPP) from of that of the benzene in *Seventh Indo-US Workshop on Mathematical Chemistry* organized by **PRIST University, TN, India and University of Minnesota, Minnesota, USA** on December 04-06, 2012 at Thanjavur-613403, Tamil Nadu, India.