

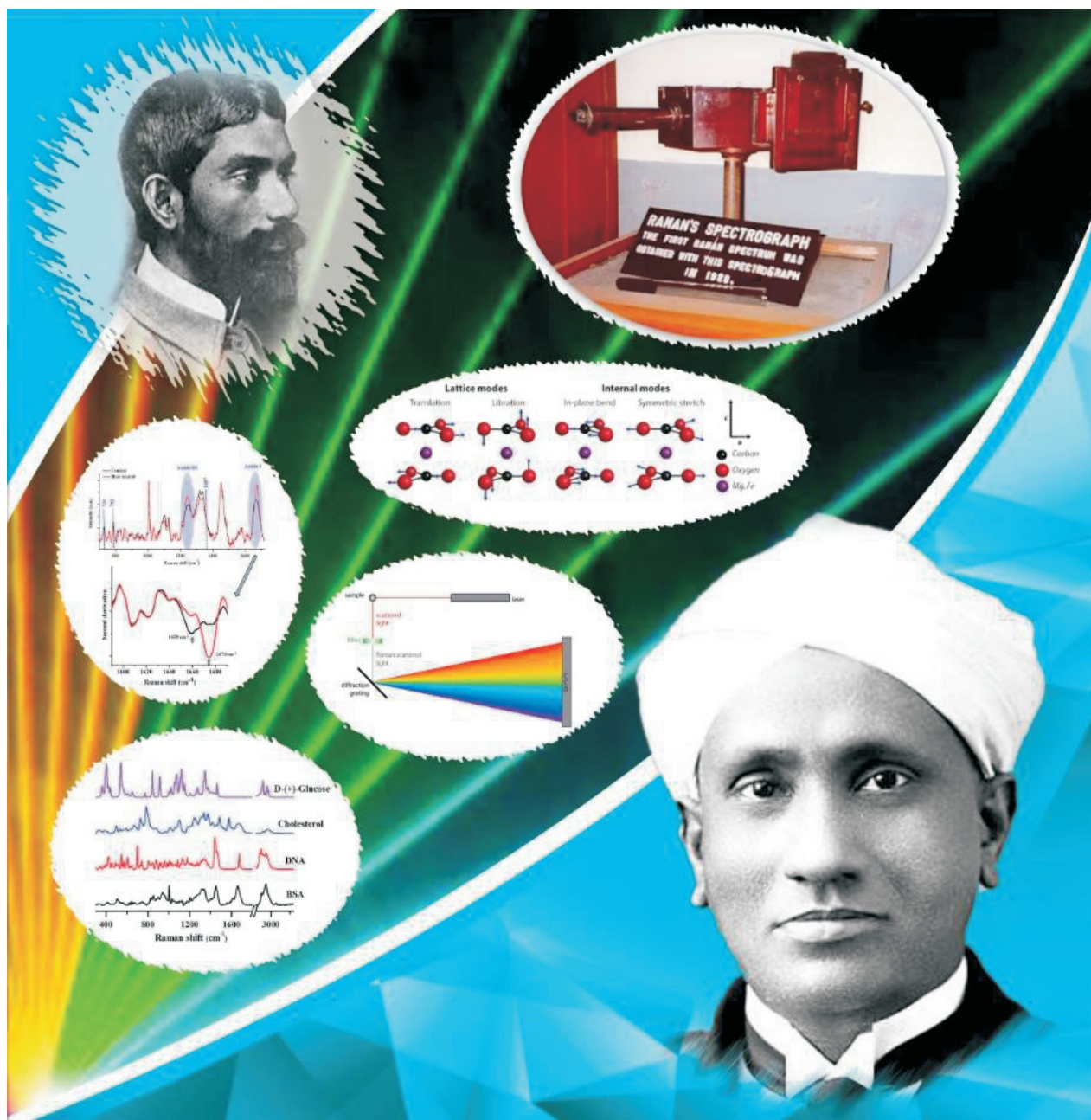
ISBN : 978-81-954339-1-9

Education in Chemical Science and Technology

Volume 9

pp. 1-154

December 2021



Published by

Indian Chemical Society

92, Acharya Prafulla Chandra Road, Kolkata - 700 009

ISBN : 978-81-954339-1-9

VOLUME 9

DECEMBER 2021

Education in Chemical Science and Technology

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The Indian Chemical Society

92, Acharya Prafulla Chandra Road, Kolkata-700 009, India

Email: ics.correspondence@gmail.com; indi3478@dataone.in

Web: <http://indianchemicalsociety.com>

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Education in Chemical Science and Technology

VOLUME 9

DECEMBER 2021

PREFACE

The 9th issue of this book series of “**Education in Chemical Science and Technology**” with twelve articles in content focusing on chemical sciences is brought out as one of the indispensable resources for the budding chemists who will choose chemistry as a coveted subject in near future.

Indian Institute of Science Education and Research (IISER) produces a host of promising scientists in different disciplines especially from Material Science Division each year. With a view to quench the thirst of the science students about IISER, Prof. Sayan Bhattacharyya *et al.* of Department of Chemical Sciences and Centre for Advanced Functional Materials, IISER, Kolkata portrays a glimpse of the IISER undergraduate curricula for Materials Science Research. In this article the various aspects of materials science and its impact particularly on renewable energy conversion and storage, environmental and healthcare applications are addressed.

The article authored by Dr. Shampa Bhattacharyya of Hansraj College, University of Delhi, describes how computer programs can be written to determine the virial coefficients through the use of least squares method using “BASIC” as a programming language. The work may benefit the undergraduate chemistry students.

Dr. Aparna Das and Prof. Bimal Krishna Banik from Departments of Mathematics and Natural Sciences, Prince Mohammad Bin Fahd University of Saudi Arabia in their exhaustive review article on “Procreation of penicillin from *Penicillium* fungi by diverse stimulants” illustrate the effect of several factors affecting the biosynthesis of penicillin by *Penicillium chrysogenum*. As claimed by the authors, the work may help the researchers to improve the production rate of antibiotics by modifying the synthesis procedures.

Dr. Himadri Sekhar Das from Department of Chemistry, Indian Institute of Engineering Science and Technology (IIST), Shibpur, in his article, depicts the zinc oxide based transparent conducting oxide thin films for different domestic and industrial applications. In the same article, the properties and importance of the film is also briefly discussed.

Bioremediation is an innovative process that uses biological sources such as microbes to remediate the heavy metals from contaminated sites. Ms. Aishwarya Das, Dr. Ranjana Das and Prof. Chiranjib Bhattacharjee of Jadavpur University studied how arsenic (As) can be bioremediated by arsenic tolerant microbes isolated from industrial soil.

Dr. Joydev Dinda, Associate Professor and Head of the Department of Chemistry, Utkal University, Bhubaneswar describes how the text book knowledge can be transmitted to the real chemical research that especially employs 'Transmetallation' and 'Disproportionation' reactions in synthesizing some biologically active metal complexes.

The article entitled "Laser and quantum optics: An emerging perception of existence" by Dr. Rajib Kumar Dubey, Haldia Institute of Technology presents the ideas and aspects of a noble laser radiation in order to obtain an insight into some topics related quantum optics and its applications.

Researchers engaged in proteomics analysis, bacterial identification, polymer chemistry and peptide chemistry etc. frequently use MALDI-TOF (Matrix Assisted Laser Desorption/Ionization-Time of Flight) mass spectrometry which is an important tool in advanced research field. Basics and applications of this modern mass spectrometry are thoroughly depicted in the contributed article of Prof. Santi M. Mandal of Indian Institute of Technology, Kharagpur.

In the present day research scenario, polymerase chain reaction (PCR) has got a momentum in the research fields of molecular biology and medical sciences in the context of the identification of pathogens in tissue sample. The present periodical depicts a piece of work on "Polymerase chain reaction (PCR)" authored by Dr. Santi M. Mandal of Indian Institute of Technology Kharagpur and his associates of different nationally reputed institutes. The article will plausibly arouse an interest among the researcher in the bio-medical field.

Prof. Animesh Kumar Rakshit in his article entitled "Negative absolute temperature: Hot or Cold" has lucidly demonstrated the class room concept of the negative absolute temperature with the help of thermodynamic definition of temperature and the Boltzmann Distribution law. This interesting short article seems to draw the attention of undergraduate and postgraduate science students.

In Ayurveda, *Swertia chirata* is being used as a traditional medicinal plant in the Indian subcontinent for treatment of diverse human ailments like stomachic, febrifuge,

antihelminthic, diuretic as well as for treatment of some types of mental disorders. Dr. Suparna Rana, Haldia Institute of Technology and Dr. Kalyan Kumar Rana, Tamralipta Mahavidyalaya jointly illustrate the medicinal efficacy of the said Ayurvedic plant in their review article.

Currently, molecular logic gates find themselves as an emerging area in frontier chemical research arena owing to their wide applications. Be it water quality monitoring or heavy metal detection or disease diagnosis and treatment or food safety detection or biological sensors, everywhere the logic operation replacing the classical silicon-based technology is acclaimed for its fast development. Prof. Chittaranjan Sinha of Jadavpur University sheds a light on how the ions/molecules can be detected at ultra trace level using chemosensors that work on 'turn-on' or 'turn-off' mechanism.

The academic contribution of all the authors who have enriched this book by sharing their valuable research articles is gratefully acknowledged. Due thanks are extended to all the Council Members and Advisors of Indian Chemical Society for their valuable inputs to bring out this issue.

Lastly, we heartfully thank the Office Staff of the Society as well as the Press for their constant cooperation in publishing this issue. Thanks are also due to Mr. Rahul Mitra, Haldia, West Bengal for designing the cover page of this issue. Notwithstanding our best efforts some mistakes might have inadvertently crept in for which we may be excused beforehand.

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IISER undergraduate curricula for Materials Science Research

Nikalabh Dihingia[#], Rachana Bhattacharyya[#] and Sayan Bhattacharyya^{*}

Department of Chemical Sciences and Centre for Advanced Functional Materials,
Indian Institute of Science Education and Research (IISER) Kolkata,
Mohanpur-741 246, West Bengal, India

[#]Equal contribution

^{*}E-mail: sayanb@iiserkol.ac.in

The purpose of this article is to portray the role of Indian Institute of Science Education and Research (IISER) system in shaping future science leaders of India, with an emphasis on materials chemistry. Starting from an overview of the expectations from science students, the article provides a glimpse of the IISER system and the 5-year BS-MS dual degree program. The various aspects of materials science and its impact are discussed, particularly based on renewable energy conversion and storage, environmental and healthcare applications. Finally, a detailed overview of the BS-MS course curriculum and its advantages in making future scientists particularly for materials chemistry research is presented.

Keywords: IISER, Science Pursuit, BS-MS Curricula, Materials Science.

Science pursuit by Indian students

High quality scientific research needs a comprehensive understanding of the what's, the how's and the whys, breaking boundaries and moving beyond the comfort zone of available knowledge. A genuine scientific research culture gets inculcated within the student at different stages, starting from high school which takes a mature shape during bachelor's and master's studies and finally acquires a direction during the doctoral studies. Just like scientific research do not obey any pre-defined boundaries between the major disciplines of biology, chemistry, physics, mathematics and/or different engineering branches, a student's mind should follow a similar pattern. The vibrant scholarly mind should never be prejudiced and to do that students need to be nurtured by thought provoking teachers and most importantly a diverse course curriculum. One such curriculum



BASIC as a programming language for undergraduate students of chemistry

Shampa Bhattacharyya

Department of Chemistry, Hansraj College, University of Delhi, Delhi-110 007, India

E-mail: shampa4@gmail.com

This article is written for the undergraduate students to learn how computer programs should be written to estimate virial coefficients through the use of least squares method using "BASIC" as a programming language. The students will be able to compare the estimated results with experimental values to find out how close they are. They can also replicate this exercise for other problems in chemistry.

Keywords: Virial coefficient, programming, least square, BASIC language, linear, non-linear.

This article demonstrates how computer programming can be applied for computing virial coefficients through the use of least squares method. The "least squares" method is a popular tool in regression analysis. It has plenty of applications in the physical chemistry. Computer programming makes computation of unknown parameters even faster and easier. In this article, the programs have been written for nonlinear and linear least squares method in "BASIC" programming language. BASIC i.e. Beginner's All Purpose Symbolic Instruction Code is a general purpose, high level programming language. This was originally designed by John G. Kemeny and Thomas E. Kurtz at Dartmouth in 1964 for students who had no prior understanding of programming¹. The software used here is QBASIC which is freely available online and can be downloaded easily. As beginners, the undergraduate students without any background in computer programming will find it simpler to understand the underlying logic in programming. The programs for both the method i.e. nonlinear least squares method (I) and linear least squares method (II) are written and provided in the Appendix at the end.

The problem which is chosen for the determination of virial coefficients meets



Procreation of penicillin from *Penicillium* fungi by diverse stimulants

Aparna Das* and Bimal Krishna Banik*

Department of Mathematics and Natural Sciences,

College of Sciences and Human Studies, Prince Mohammad Bin Fahd University,

Al Khobar 31952, Kingdom of Saudi Arabia

*E-mail: aparnadasam@gmail.com, bimalbanik10@gmail.com, bbanik@pmu.edu.sa

Penicillium fungi are a foundation for a large pharmaceutical industry of antibiotics. A group of antibiotics called Penicillin is derived from *Penicillium* fungi. Synthesis of penicillin antibiotics is traditionally important since these antibiotics are the first drugs that were effective against several serious diseases. Penicillin can be extracted from *Penicillium notatum* or *Penicillium chrysogenum*. However, *Penicillium chrysogenum* is the main fungal species used for the production of penicillin. The secretion of metabolites in *Penicillium chrysogenum* can be affected by several factors. In view of the importance of penicillin synthesis from *Penicillium chrysogenum* in the field of industry and medicine, the current review aims to describe the effects of different synthetic constituents on the penicillium productivity by *Penicillium chrysogenum*.

Keywords: Penicillin, antimicrobial, biosynthesis, natural product, *Penicillium*, antibiotics.

1. Introduction

A large number of microorganisms are used for the synthesis of antibiotics. Among them, *Penicillium* is a foundation for a large pharmaceutical industry of antibiotics. A group of antibiotics called Penicillin (PCN or PEN) is derived from *Penicillium* fungi. This antibiotic group includes many compounds such as Penicillin G, Penicillin V, Procaine penicillin, and Benzathine penicillin (Fig. 1). Structurally, all penicillins are β -lactam antibiotics. Over the past decade, the synthesis and biological activities of β -lactams derivatives have been widely studied by our group¹⁻⁵. Synthesis of penicillin antibiotics is traditionally important since these antibiotics are the first drugs that were effective against



Zinc oxide based transparent conducting oxide thin films for different domestic and industrial applications

Himadri Sekhar Das

Department of Chemistry, Indian Institute of Engineering Science and Technology (IIST),
Shibpur-711 103, West Bengal, India

E-mail: das.himadrisekhar@gmail.com, himadrisekhar_das@rediffmail.com

Thin films consist of a very thin layer of 10 nm to 2 μm of material deposited on different substrate such as glass, silicon wafer, polymer. Thin films are deposited in optimized conditions like inert gas, pressure, duration, substrate temperature by a physical or chemical process. Transparent conducting oxide (TCO) also belongs to the thin film category. Different type TCO materials are available among them ITO, SnO_2 are commercially established TCO materials and different doped (boron (B), aluminum (Al), gallium (Ga), indium (In) or fluorine (F)) ZnO film are also used as TCO materials. ZnO has been promoted as a promising II-VI semiconductor material for a TCO layer for photovoltaic applications less expensive than tin and indium, band gap 3.4 eV, large exciton binding energy (60 meV), large piezoelectric constant, resource availability, strong luminescence, high thermal conductivity, amenability to wet chemical etching, radiation hardness, easy surface texturing method, stability in hydrogen plasma and non-toxicity also fabrication of high quality single crystal and epitaxial layer zinc oxide shows developed growth technologies allowing for the realization of ZnO-based applications like electronic and optoelectronic devices.

In this article a brief discussion was made on Zinc Oxide based transparent conducting oxide thin film properties and preparation for different domestic and industrial applications.

Keywords: ZnO, TCO, OLED, solar cell, thin-film transistor, display, gas sensors.

Introduction

A thin film can be defined as a very thin layer of 10 nm to 2 μm of material deposited on a substrate like glass, silicon wafer, polymer etc. by the optimized parameter such as inert gas, pressure, duration, substrate temperature by a physical or chemical process. This technology is known as thin film technology.



Microbial bioremediation of arsenic by arsenic tolerant bacteria isolated from industrial soil

Aishwarya Das, Ranjana Das* and Chiranjib Bhattacharjee

Chemical Engineering Department, Jadavpur University,
Kolkata-700 032, India

*E-mail: ranjanads78@gmail.com, ranjana.das@jadavpuruniversity.in

Heavy metals are typically categorized as unavoidable contaminants of environment and arsenic is most crucial heavy metal of concern. Arsenic appears in nature in different oxidation state and trivalent one, As(III) is reported as the component responsible for toxicity to animal and human as this form is more persistent in nature and cannot be broken down completely in non-toxic form. Bioremediation is a process that uses biological sources such as microbes to remediate the heavy metals from contaminated sites. The present study aims to introduce the concept of microbiology to neutralize/eliminate the toxicity of As(III). Seven bacteria were isolated from two soil sample collected from the industrial zone of district Howrah and district South 24-Parganas, West Bengal. The MIC values of the isolated bacterial systems experimentally observed and a consortium was prepared based on MIC values to achieve optimum removal efficiency. The consortium was found to tolerate up to 200 mM of As(III) concentration and highest arsenic removal potency of 92% was observed. The plasmid DNA isolation and degradation was also performed to confirm the presence of desired genes promoting survival of the bacteria in stress conditions. Hence, with proper design and tuning, the isolates bioremediation of As(III) contaminated effluents may be achieved with immense societal benefits.

Keywords: Bioremediation, heavy metal, arsenic, microbes, industrial soil, plasmid.

1. Introduction

The indiscriminate release of the heavy metal into the soil and water is a major health concern worldwide, as it cannot be broken down into non-toxic form and therefore has long lasting effects on ecosystem¹.

Arsenic is a metalloid element, toxic in nature, which is widely distributed on surface of the earth due to natural calamities and anthropogenic activities.



Transformation of text book knowledge to real chemical research in light of 'Transmetallation' and 'Disproportionation' reactions

Joydev Dinda

Department of Chemistry, Utkal University,
Bhubaneswar-751 004, Odisha, India

E-mail: joydevdinda@gmail.com

'I hear and I forget.

I see and I believe.

I do and I understand'—

Confucius (551-479 BCE).

Silver(I)-NHC transmetallation reactions have a lot of opportunity to synthesize several other types of metal-NHC complexes. Ag(I)-NHC complexes can be used to synthesize Au(I)-, Cu(I)-, Au(III)-, Pd(II)-, Pt(II)-, Ru(II) etc. -NHC complexes which have ample of applications. Ag(I)-, Au(I)-, Cu(I)-, Au(III)-, Pd(II)-, Pt(II)-, and Ru(II)-NHC complexes may be used as potent antibacterial and anticancer drugs. On the other hand, Au(I/III)-, Pd(II)- and Ru(II)-NHC Au(I) complexes have been used as catalysts in several catalytic reactions. Disproportionation reactions pathway may be capitalized to synthesize Au(III)-NHC complexes, in this pathway use of noxious Cl_2 gas may be avoided. Applying the text book knowledge of transmetallation and disproportionation reactions a series of catalytically sound and biologically active metal-NHC complexes may be obtained experimentally.

Keywords: Transmetallation reactions, disproportionation reactions, silver(I)-NHC, gold(I/III)-NHC, anticancer activites.

Introduction

Addition, elimination, substitution, rearrangement, photochemical, radical, redox, etc. are the common reactions in organic chemistry¹. In inorganic chemistry, oxidation-reduction, precipitation reactions are very common along with elimination, substitution, photochemical, radical reactions². Inorganic



Laser and quantum optics: An emerging perception of existence

Rajib Kumar Dubey

School of Applied Science and Humanities, Haldia Institute of Technology,
Haldia-721 657, West Bengal, India

E-mail: dubeyassam@gmail.com

The historical developments of ideas associated with laser and quantum optics leads us to think that light plays such an integral part in the life of man that its nature has certainly been a source of wonder and thought throughout the civilization. Although research has progressed rapidly during this century the foundation of what we know about light, optics, quantum optics and laser indeed go back down the civilization. Different theories and ideas regarding light have been put forward by great philosophers in the past and present. Some basic things are certain to change in future. This article gives a brief introduction about the developments in the laser and quantum optics.

Keywords: Quantum optics, quantum interference lasing without population inversion (LWI), quantum Zeno effect, electromagnetic induced transparency and self induced transparency.

Introduction

Einstein in 1917 wrote “for the rest of my life I shall reflect on what light is”. Perhaps Einstein gave this statement after he worked out the famous black body radiation formula on the basis of the idea of stimulated emission. The nature and properties of light and in fact everything we know about light comes from its interaction with matter. This interaction can be explained on the basis of quantum mechanics. A clear understanding of the physical constitution of light and of the phenomena resulting from its interaction with matter is therefore essential for any valid interpretation of the facts. When an atomic system interacts with light, it can amplify the light or electromagnetic radiation when gain exceeds the loss. This also requires that transitions from upper level to the lower level prevail over the transitions from lower level to the upper level. If one deals with two level sys-



MALDI-TOF Mass spectrometry: Basics and application

Santi M. Mandal

Central Research Facility, Indian Institute of Technology Kharagpur,
Kharagpur-721 302, West Bengal, India

E-mail: mandalsm@gmail.com

MALDI-TOF-MS is an analytical technique that involves ionizing particles, sorting them based on their mass-to-charge ratio, and measuring the time it takes for the ions to travel to a detector. MALDI-TOF-MS is useful not only for resolving a chemical backbone of a compound but also for overcoming a number of challenges in clinical microbiology using a reasonably simple and rapid method. Principle, sample preparation process, and application of MALDI-TOF-MS are explained here, which is widely used in bio-molecule characterization and identification.

Keywords: MALDI-TOF-MS, Principle, application, sample preparation protocol.

First mass spectrometer was originated with the term parabola spectrograph. It was constructed first time in 1912 by J. J. Thomson after the discovery of electron in 1897. Thomson's protege, Francis Aston, has been developed a mass spectrometer where ions were dispersed and considered their velocity, showed improved over Premier Thomson's device. Further, it has been taken several more decades for the innovation of TOF-MS as an analytical tool. The first TOF instruments were designed and constructed in the late 1940s, and the Bendix Corporation in Detroit. MALDI-TOF (Matrix Assisted Laser Desorption/Ionization-Time of Flight) is routinely used for proteomics analysis, bacterial identification, polymer chemistry and peptide chemistry etc. It is widely used to characterize and identify the analyte mixtures of organic molecules.

There are three major components of MALDI mass spectrometry:

(i) Ion source: Ion source by which the samples are ionized. There are several types of ionization process used in mass spectrometry methods. In 1st generation mass spectrometry, the electron impact (EI) and Fast Atom Bombardment (FAB) was very flattering technique. These techniques are not



Polymerase chain reaction (PCR)

**Santi M. Mandal^{*a}, Gourisankar Roymahapatra^b, Debarati Paul^c,
D. Madhusudan Reddy^c and Christine Jeyaseelan^c**

^aCentral Research Facility, Indian Institute of Technology Kharagpur,
Kharagpur-721 302, West Bengal, India

^bSchool of Applied Science and Humanities, Haldia Institute of Technology,
Haldia-721 657, West Bengal, India

^cDepartment of Biotechnology, Department of Microbiology, Department of Chemistry,
Amity University, Noida-201 301, Uttar Pradesh, India

**E-mail:* mandalsm@gmail.com

The polymerase chain reaction (PCR) is a method for amplifying DNA sequences millions or billions of times. This technique is accomplished with three major steps is denaturation or separation of the two strands of the DNA, annealing of primers, and extension of the new DNA strands from the primers. After each cycle, the numbers of copies become doubles. The principle, types, and applications of PCR have been thoroughly summarized here. It enables us to investigate that DNA molecule in more depth in the laboratory and is commonly employed in DNA cloning, medical diagnostics, and forensic DNA analysis.

Keywords: PCR, DNA amplification, steps, medical diagnosis.

Polymerase chain reaction (PCR) is a widely used method in molecular biology and medical sciences to increase the copy number of specific DNA segment or identify the pathogens in tissue sample. PCR is the most pioneer technique in molecular biology and most fascinating useful techniques in medical sciences. PCR has enormous practical applications in the field of biology, medicine, molecular biology, research etc. PCR was invented by Kary Mullis in 1983. This technique is an efficient, highly valuable, inexpensive and most reliable technique. It is used in common laboratory practices to amplify small fragments of DNA to large amount of DNA fragments following a universal protocol as follows^{1,2}:



Negative absolute temperature: Hot or Cold

Animesh Kumar Rakshit

47/1 Ghosh Para, Flat 301, Haltu, Kolkata-700 078, India

E-mail: akrakshi@yahoo.co.in

Absolute (Kelvin) temperature is always considered positive. However, from thermodynamics the presence of negative absolute temperature is quite obvious. In this short article it is suggested that this fact be brought to the attention of undergraduate and postgraduate chemistry students.

Keywords: Thermodynamics, nuclear spin, negative temperature, population inversion, Hot, Cold.

In teaching Thermodynamics to undergraduate and postgraduate students of chemistry in India, the concept of negative absolute temperature is, in general, not introduced or discussed. The second law of thermodynamics is normally introduced with the implicit assumption that absolute temperature can never be negative. The third law of thermodynamics states: it is impossible to attain absolute zero in a finite number of operations. This is also known as the "principle of un-attainability of absolute zero". The lowest temperature of zero degree absolute is, therefore, unattainable. Though this is true for practical situation/importance, the concept of negative absolute temperature is of importance and use in the understanding of the theory behind the production of "masers" and "lasers" that result from "population inversion". Therefore, a clear introduction of the concept ought to be a requirement for the students.

To introduce the negative absolute temperature we should consider (i) the thermodynamic definition of temperature, and (ii) the Boltzmann Distribution law. The combined first and second laws of thermodynamics can be written as

$$TdS = dU + PdV,$$

where the symbols have their usual significance. At constant volume,

$$T = (dU/dS)_V = (dS/dU)_V^{-1}.$$

The absolute temperature is thus defined as the inverse of the rate of change of entropy per unit change of internal energy. We can also write,



Medicinal efficacy of *Swertia chirata* buch-ham revisited

Suparna Rana^a and Kalyan Kumar Rana^{*b}

^aSchool of Applied Science and Humanities, Haldia Institute of Technology,
Haldia-721 657, West Bengal, India

^bDepartment of Chemistry, Tamralipta Mahavidyalaya, Tamluk-721 636,
West Bengal, India

*E-mail: kalyankrana@yahoo.co.in

Swertia chirata is a plant with bitter taste used since remote past in traditional medical systems in the Indian subcontinent for treatment of diverse human ailments. In Ayurveda, the plant is used as stomachic, febrifuge, antihelminthic, diuretic as well as for treatment of some types of mental disorders. Experimental confirmation of the usefulness of this plant along with chemical analyses of its constituents have created much interest in the screening of medicinal value of *Swertia chirata* and is likely to expose new opportunities for its multispectral exploitation. In view of the antioxidative, anti-inflammatory and anticarcinogenic activities, the plant deserves a more detailed exploration to find out its use in pharmaceutical industry for preparation of remedies towards prevention and treatment of acute and chronic human diseases.

Keywords: *Swertia chirata*, Ayurveda, antioxidative, anti-inflammatory, antimalarial, antihepatotoxic, antihelminthic.

1. Introduction

Traditional and alternative medicine is becoming gradually more popular and experiencing a high expansion all over the world. The medicinal plant, *Swertia chirata*, has been widely used as herbal medicine in Asian countries from time immemorial. It was first described by Roxburgh under the name of *Gentiana chyrayta*¹ in 1814. The herb is much appreciated by the Ayurvedic physicians because of its febrifuge, antihelminthic, tonic and laxative properties. The word *chirata* or *chirayata* comes from the Sanskrit *Kirata*, name of a mountain tribe of hunters that lives on high mountains, in preferably wooden houses. They are the *Shudras* (the members of the fourth or last social group of Hindu caste system) because they may or may not be Hindus but follow an animistic (the belief in the



Molecular logic gate

Chittaranjan Sinha

Department of Chemistry, Jadavpur University, Kolkata-700 032, India

E-mail: crsjuchem@gmail.com

Molecular logic gate is a part of Boolean algebra. It is mostly used in circuitary motif which runs through binary operation of two variables '0' and '1'. In molecular sensing this project shows outstanding application. The chemosensors in our laboratory are designed for the detection of ions/molecules at ultratrace level and follows 'turn-on' or 'turn-off' mechanism that is a two-variable system.

Keywords: Boolean Algebra, binary operation, ion and molecular sensing, turn-on, turn-off, trace level detection.

1. Logic operation : Boolean algebra

Boolean logic deals with binary operation of two variables only, 1 and 0 by which all the mathematical operations are to be performed. Three basis binary operations, AND, OR, and NOT are used by which all simple, as well as complex binary mathematical operations, are to be addressed¹. Besides, some derived operation such as NAND, NOR, EX-OR, EX-NOR are also performed with same mathematics. In Boolean algebra, the variables are represented by English Capital Letter like A, B, C, etc. and the value of each variable can be either 1 or 0, nothing else.

Some basic laws for Boolean algebra

$A \cdot 0 = 0$ where A can be either 0 or 1.

$A \cdot 1 = A$ where A can be either 0 or 1.

$A \cdot A = A$ where A can be either 0 or 1.

$A \cdot \bar{A} = 0$ where A can be either 0 or 1.

$A + 0 = A$ where A can be either 0 or 1.

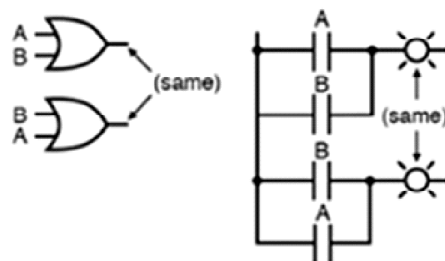
$A + 1 = 1$ where A can be either 0 or 1.

$A + \bar{A} = 1$

$A + A = A$

Commutative Property of Addition

$$A + B = B + A$$



ISBN : 978-81-954339-1-9



"While a student at Edinburgh I found to my regret that every civilized country including Japan was adding to the world's stock of knowledge but unhappy that India was lagging behind. I dreamt a dream that, God willing, a time would come when she too would contribute her quota. Half-a-century has since then rolled by. My dream I have now the gratification of finding fairly materialized. A new era has evidently dawned upon India. Her sons have taken kindly to the zealous pursuit of different branches of science. May the torch thus kindled burn with greater brilliance from generation to generation "

Acharya Profulla Chandra Ray

All correspondences should be addressed to :

Professor Chittaranjan Sinha

Honorary Secretary
Indian Chemical Society
92, Acharya Profulla Chandra Road
Kolkata-700 009

E-mail : ics.correspondence@gmail.com
indi3478@dataone.in

Web : <http://www.indianchemicalsociety.com>

Fax-o-Phone : 91-033-23503478

Phone : 91-033-23609497

Price : ₹ 200.00

Published by the Honorary Secretary on behalf of Indian Chemical Society, 92, Acharya Profulla Chandra Road, Kolkata-700 009, India,
and Printed at Auto-Print & Publicity House, 49, Baldeopara Road, Kolkata-700 006, India