INDIAN INSTITUTE OF TECHNOLOGY PATNA

THC TRIBUNE

Vol. 7

A MAGAZINE FOR CHEMICAL COMMUNITY

Magazine Fabricated by :
Divyanshu Khandelwal
Mar 19, 2017

Contents

List of Figures

1 ALL AROUND THE WORLD

1.1 Catalytic reaction also reduces pollution!!

A research team has improved an important catalytic reaction commonly used in the oil and gas industries. The innovation could lead to dramatic energy savings and reduced pollution, they say.
Link : https://www.sciencedaily.com/releases/2017/02/170227125159.htm

1.2 Triboelectric nanogenerators boost mass spectrometry performance !!

Triboelectric nanogenerators (TENG) convert mechanical energy harvested from the environment to electricity for powering small devices such as sensors or for recharging consumer electronics. Now, researchers have harnessed these devices to improve the charging of molecules in a way that dramatically boosts the sensitivity of a widely-used chemical analysis technique.
Link: https://www.sciencedaily.com/releases/2017/02/170227120234.htm

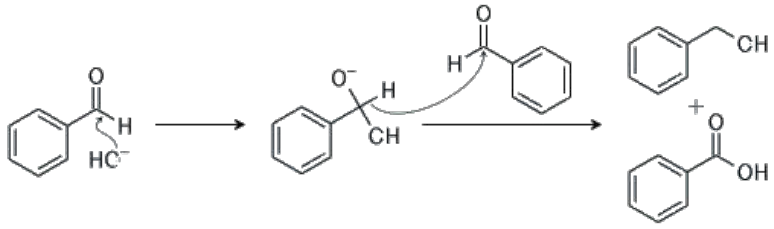
1.3 Materials that emit rainbows!!

Mechanochromic luminescent (MCL) materials change their color in response to a change in their environment, like pressure and temperature. To date, most MCL materials only change between two colors, limiting their applications. A international research team has developed tricolor-changing MLC materials. Not only that, the developed materials exhibited efficient thermally activated delayed fluorescence (TADF) and allowed high performance organic light-emitting diodes (OLEDs) devices.
Link : https://www.sciencedaily.com/releases/2017/02/170227082524.htm

2 LEARNING ZONE

2.1 Reaction you must know

The Cannizzaro reaction, named after its discoverer Stanislao Cannizzaro, is a chemical reaction that involves the base-induced disproportionation of an aldehyde lacking a hydrogen atom in the alpha position.



Cannizzaro first accomplished this transformation in 1853, when he obtained benzyl alcohol and potassium benzoate from the treatment of benzaldehyde with potash (potassium carbonate). More typically, the reaction would be conducted with sodium or potassium hydroxide:

$$2\ C_6H_5CHO + KOH \longrightarrow C_6H_5CH_2OH + C_6H_5COOK$$

The oxidation product is a salt of a carboxylic acid and the reduction product is an alcohol.

The reaction involves a nucleophilic acyl substitution on an aldehyde, with the leaving group concurrently attacking another aldehyde in the second step. First, hydroxide attacks a carbonyl. The resulting tetrahedral intermediate then collapses, re-forming the carbonyl and transferring hydride to attack another carbonyl. In the final step of the reaction, the acid and alkoxide ions formed exchange a proton. In the presence of a very high concentration of base, the aldehyde first forms a doubly charged anion from which a hydride ion is transferred to the second molecule of aldehyde to form carboxylate and alkoxide ions. Subsequently, the alkoxide ion acquires a proton from the solvent.

3 INFORMATION ZONE

3.1 Bharat Petroleum Corporation Ltd

BPCL is a Fortune 500, leading Navratna Public Sector Company. It is a well known PSU in the energy sector engaged in Refining, Marketing and Distribution of Petroleum products and also in exploration of Oil / Gas. The BPCL group achieved a Gross Revenue from Operations of Rs. 2,19,253.07 crores for the year 2015-16. BPCL recruitment of graduate engineers at the entry level has been for the past few years through GATE scores.

Eligibility for BPCL Recruitment through GATE 2017

BPCL Eligibility Parameters	**Details**
Nationality	Indian Nationals Only
Academic Qualifications	Candidates must have pass a 4 year full time B.Tech/ B.E or equivalent from a recognized Institute or University. Final year candidates can apply provided they furnish proof of their eligibility by August 31, 2017.
Pass percentage of Qualifying Degree	They must have obtained a minimum of 60 percent in aggregate in their degree. SC/ST candidates have relaxation up to 55 percent.

Selection Process for BPCL Recruitment through GATE

Stages of Selection Process	Parameters
Shortlisting	On the basis of valid GATE-2017 Scores
Further Shortlisting on the basis of performance in	Group Discussions / Alternate selection methodology Personal Interviews
Selection	Based on Medical Fitness in Pre -Employment Medical Examination

GATE Cutoff for BPCL Recruitment of previous years

Applicants can check the cutoffs for the BPCL Recruitment through GATE for the previous below to get an idea of the GATE marks that are needed to be shortlisted and called for the further interview process.

GATE 2016 Cutoff for BPCL Recruitment

Branch	GEN	OBC	SC	ST
Mechanical	68	65	54	46
Chemical	57	55	47	40
Instrumentation	60	58	43	33

Probation and Training : Candidates will be selected as Management Trainee placed in Job Group A. The probation period will be one year which may be extended in case of non-satisfactory performance.

After Probation: Candidates who have successfully completed their probation will be absorbed as Executive in the respective business unit/entity.

Posting Area: The posting of candidates may be at any of the BPCL offices across the country and this will be at the discretion of the company.

Work Profile: Candidates may be posted in Operations, Sales and Process and Engineering at refineries. Candidates posted in Operations may be required to work in shifts.

Salary Details

Pay Scale: Candidates will be paid a basic salary of Rs. 24,900/- with the pay scale being Rs. 24,900 Rs. 50,500 plus Dearness Allowance (DA) based on IDA pattern. The House Rent Assistance, if applicable will depend on the class of city of posting.

Cost to Company: Rs.10.5 lakhs per annum which is due for an upward revision in 2017 and effective from January 1, 2017. This includes 50 percent of Basic Pay as Perks and Allowances, Performance Related Pay. It is inclusive of 30 percent of Basic plus DA as superannuation benefits (Provident Fund, Gratuity and New Pension Scheme). Other perquisites payable include housing / vehicle loan facilities, medical reimbursement for candidate / dependant family members, LFA, Holiday home facility, Group Savings Linked Insurance Scheme etc.

4 EXPLORE ZONE

4.1 Nuclear Chemistry

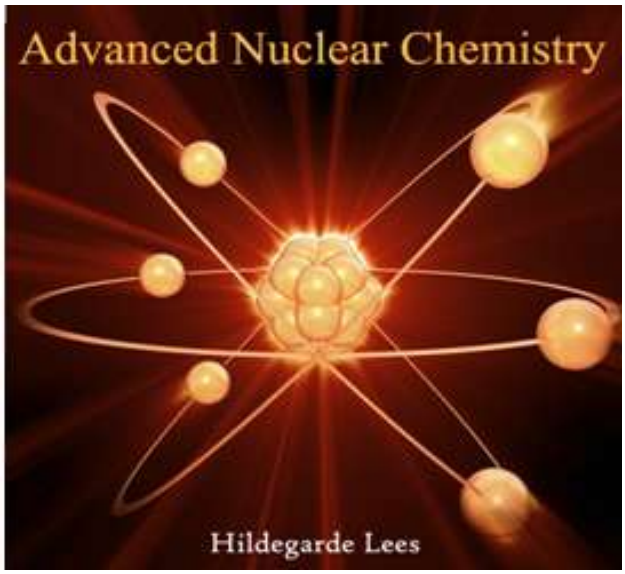


Figure 1: Nuclear Chemistry

Nuclear chemistry is the subfield of chemistry dealing with radioactivity, nuclear processes, such as nuclear transmutation, and nuclear properties.

It is the chemistry of radioactive elements such as the actinides, radium and radon together with the chemistry associated with equipment (such as nuclear reactors) which are designed to perform nuclear processes. This includes the corrosion of surfaces and the behavior under conditions of both normal and abnormal operation (such as during an accident). An important area is the behavior of objects and materials after being placed into a nuclear waste storage or disposal site.

It includes the study of the chemical effects resulting from the absorption of radiation within living animals, plants, and other materials. The radiation chemistry controls much of radiation biology as radiation has an effect on living things at the molecular scale, to explain it another way the radiation alters the biochemicals within an organism, the alteration of the biomolecules then changes the chemistry which occurs within the organism, this change in chemistry then can lead to a biological outcome. As a result, nuclear chemistry greatly assists the understanding of medical treatments

(such as cancer radiotherapy) and has enabled these treatments to improve.

It includes the study of the production and use of radioactive sources for a range of processes. These include radiotherapy in medical applications; the use of radioactive tracers within industry, science and the environment; and the use of radiation to modify materials such as polymers. It also includes the study and use of nuclear processes in non-radioactive areas of human activity. For instance, nuclear magnetic resonance (NMR) spectroscopy is commonly used in synthetic organic chemistry and physical chemistry and for structural analysis in macromolecular chemistry.

A combination of radiochemistry and radiation chemistry is used to study nuclear reactions such as fission and fusion. Some early evidence for nuclear fission was the formation of a short-lived radioisotope of barium which was isolated from neutron irradiated uranium (139Ba, with a half-life of 83 minutes and 140Ba, with a half-life of 12.8 days, are major fission products of uranium). At the time, it was thought that this was a new radium isotope, as it was then standard radiochemical practice to use a barium sulfate carrier precipitate to assist in the isolation of radium. More recently, a combination of radiochemical methods and nuclear physics has been used to try to make new 'superheavy' elements; it is thought that islands of relative stability exist where the nuclides have half-lives of years, thus enabling weighable amounts of the new elements to be isolated.

5 LET'S TALK CHEMISTRY

5.1 Chemistry in everyday life

The history behind your eraser

An eraser is an instrument of stationery used to remove pencil and sometimes pen marks. It is rather interesting to know that before the invention of erasers slabs of wax and breadcrumbs were used to 'wipe out' charcoal or lead marks from paper. Can you imagine doing that in the classroom? The first pencils were discovered around 1560's but people did not have anything that could rub out the marks with.

The first erasers

The history of the first erasers dates back all the way back to 1770 when Joseph Priestley discovered a vegetable gum that possessed the ability to 'rub out' pencil marks. Quite similarly, in the same year, Edward Nairne, an English engineer discovered rubber's erasing properties. This was the first practical use of the substance in the whole of Europe.

When the facts don't stretch

It was noticed that while the rubber softened in warm weather, it became hard in cold conditions. What 's more, the first rubbers had an unpleasant smell if you kept using it. A scientist named Charles Goodyear invented the process of 'vulcanization' in 1839. This innovative process enabled rubber to become more long lasting, elastic and more durable in nature.

Charles Goodyear invented the process of 'vulcanization' in 1839

Different types of erasers are made up of various raw materials, each with similar properties and a suited application. Erasers are examples of polymers and possess certain elasticity, a suitable property for "rubbing' or 'erasing'. Erasers can be made up of myriad materials such as vinyl, gum, and rubber, plastic, and synthetic rubber.

How an eraser makes everything disappear

Ever wondered how all these materials erase graphite, charcoal and lead marks on paper? The logic behind it is quite simple. The molecules in erasers are relatively stickier than those constituting paper. Therefore, when an eraser is rubbed onto a pencil mark, the graphite sticks to the eraser's surface instead of the paper's surface. While it does this, the eraser can damage the top layer of the paper itself if used too roughly. It leaves some residue on the paper, which then needs to be removed. Erasers are primarily adsorbents.

The different types of erasers

Modern erasers can be made into various shapes sizes and colors. Some of the types of erasers used today are the plug erasers, the kneaded erasers, the art gum erasers and the white vinyl erasers. Plug erasers are those found at the back of a pencil on the opposite side of the graphite tip, whereas kneaded erasers function by absorbing or picking graphite particles and are sticky in nature like chewing-gum. These erasers do not disintegrate nor do they leave behind any eraser residue and hence last much longer.

Kneaded erasers can be moulded into any shape and employed for precision erasing. Vinyl erasers are the white ones that are most commonly used and are soft in nature. These erasers are plastic like in texture and erase more cleanly as compared to the normal pink eraser.

6 NOBEL LAUREATES IN CHEMISTRY

DAN SHECHTMAN GOT NOBEL PRIZE IN CHEMISTRY IN 2011 FOR THE DISCOVERY OF QUASICRYSTALS

Figure 2: Dan Shechtman

In quasicrystals, we find the fascinating mosaics of the Arabic world reproduced at the level of atoms: regular patterns that never repeat themselves. However, the configuration found in quasicrystals was considered impossible, and Dan Shechtman had to fight a fierce battle against established science. The Nobel Prize in Chemistry 2011 has fundamentally altered how chemists conceive of solid matter.

On the morning of 8 April 1982, an image counter to the laws of nature appeared in Dan Shechtman's electron microscope. In all solid matter, atoms were believed to be packed inside crystals in symmetrical patterns that were repeated periodically over and over again. For scientists, this repetition was required in order to obtain a crystal.

Shechtman's image, however, showed that the atoms in his crystal were packed in a pattern that could not be repeated. Such a pattern was considered just as impossible as creating a football using only six-cornered polygons, when a sphere needs both five- and six-cornered polygons. His

discovery was extremely controversial. In the course of defending his findings, he was asked to leave his research group. However, his battle eventually forced scientists to reconsider their conception of the very nature of matter.

Aperiodic mosaics, such as those found in the medieval Islamic mosaics of the Alhambra Palace in Spain and the Darb-i Imam Shrine in Iran, have helped scientists understand what quasicrystals look like at the atomic level. In those mosaics, as in quasicrystals, the patterns are regular - they follow mathematical rules - but they never repeat themselves.

When scientists describe Shechtman's quasicrystals, they use a concept that comes from mathematics and art: the golden ratio. This number had already caught the interest of mathematicians in Ancient Greece, as it often appeared in geometry. In quasicrystals, for instance, the ratio of various distances between atoms is related to the golden mean.

Following Shechtman's discovery, scientists have produced other kinds of quasicrystals in the lab and discovered naturally occurring quasicrystals in mineral samples from a Russian river. A Swedish company has also found quasicrystals in a certain form of steel, where the crystals reinforce the material like armor. Scientists are currently experimenting with using quasicrystals in different products such as frying pans and diesel engines.

7 RESEARCH BY PROFESSORS AT IITP

Hierarchical coassembly of DNAtriptycene hybrid molecular building blocks and zinc protoporphyrin IX

This is one of the project work of Associate Professor Mr. Prolay Das along with the research scholars Rina Kumari, Sumit Singh, Mohan Monisha, Sourav Bhowmick, Anindya Roy.

Figure 3: Prolay Das

Abstract

Herein, we describe the successful construction of composite DNA nanostructures by the self-assembly of complementary symmetrical 2,6,14-triptycenetripropiolic acid (TPA)DNA building blocks and zinc protoporphyrin IX (Zn PpIX). DNAorganic molecule scaffolds for the composite DNA nanostructure were constructed through covalent conjugation of TPA with 5-C12-amine-terminated modified single strand DNA (ssDNA) and its complementary strand. The repeated covalent conjugation of TPA with DNA was confirmed by using denaturing polyacrylamide gel electrophoresis (PAGE), reverse-phase high-performance liquid chromatography (RP-HPLC) and matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF). The biologically relevant photosensitizer Zn PpIX was used to direct the hybridization-mediated self-assembly of DNATPA molecular building blocks as well as a model guest molecule within the DNATPA supramolecular self-assembly. The formation of fiber-like composite DNA nanostructures was observed. Native PAGE, circular dichroism (CD) and atomic force microscopy (AFM) have been utilized for analyzing the formation of DNA

nanofibers after the coassembly. Computational methods were applied to discern the theoretical dimension of the DNATPA molecular building block of the nanofibers. A notable change in photocatalytic efficiency of Zn PpIX was observed when it was inside the TPADNA scaffold. The significant increase in ROS generation by Zn PpIX when trapped in this biocompatible DNATPA hybrid nanofiber may be an effective tool to explore photodynamic therapy (PDT) applications as well as photocatalytic reactions.

Conclusion

A novel DNAorganic hybrid molecule has been synthesized by the covalent coupling of amine-terminated DNA with TPA. Characterization of the DNATPA hybrids by denaturing PAGE, RP-HPLC and MALDI-TOF analysis showed the formation of all three possible products in which TPA was conjugated with either one, two or three ssDNA. The rigid framework of TPA is expected to produce scaffolds for the biologically relevant molecule (Zn PpIX) after conjugation and assembly with DNA complementary strands. Interestingly, coassembly of DNATPA building block units and Zn PpIX generates DNA nanofibers showing enhanced photocatalytic activity. These features have been identified and confirmed by native PAGE, AFM, CD and spectroscopic analyses. It was observed that tri-conjugated hybrid units are self-assembled into small oligomeric products leading to unorganized structures in the absence of Zn PpIX where as higher-order organized structures with B-form conformation of DNA were seen in the presence of Zn PpIX. Although, the TPA moiety offers 120 angular disposition of the ssDNA strands after conjugation, tetrameric building blocks are still formed due to the inherent flexibility of the DNA duplex after self-assembly.

It can be concluded that the Zn PpIX re-equilibrate the self-assembled mixture into the selected nanostructures, thus providing an additional level of control in DNA structuring. Our experiments point out to the fact that Zn PpIX redirects the self-assembly and initiates the formation of ordered structures.Hierarchical coassembly of DNAtriptycene hybrid molecular building blocks and zinc protoporphyrin IX.

8 Q AND A ZONE

Welcome back readers!! Today we have with us Ms. Pranjali Sharma (Pre final year student), one of the best examples of hardworkers in our college (so called 10 pointer) . She shared her internship experience of IIT INDORE in a small chat with us.

ThC: Please tell us about the project work you did.

Pranjali: The project work I did in my research intern , last year at IIT, Indore comprised of Asymmetric synthesis of optically active compounds. I dealt with green organic synthesis under the project title: Highly Diastereoselective One-pot synthesis of densely functionalized Tetrahydrocarbazoles catalyzed by organobases. The use of this research work is in the synthesis of Tetrahydrocarbazoles (used in pharmaceutical industry) which have eight optically active carbon centres. So after the synthesis we had chances of getting 28 products. This leaded to low yield of the desired product. The method we used to synthesise these tetrahydrocarbazoles used Michael and Henry reactions to form highly diastereoselective product using indole and its derivatives . The synthesis involved doing the desired reaction at milligram scale and separating the desired product from the unreacted compounds and other impurities using column chromatography. After one complete synthesis the compounds were resynthesised using different substituent on the basic reactant i.e. the indole derivative (indolene) . After each synthesis the obtained product was characterized using NMR Spectroscopy and Mass Spectrometry . The reaction yield was analysed as the substituents changed i.e. ERGs and EWGs.

ThC: How did you manage to get an internship in 2nd year? Tell us about the problems you faced while applying?

Pranjali: I didnt had any plans to do an intern in the summers of my second year until I met a friend of my dad, who explained me the benefits of doing an intern, a research intern to be specific in my case. It was the ending of May by then, so I thought that getting an intern might be impossible, as most of my friends I knew had joined their labs way back. I started mailing some professors whom I knew personally or who were friends of my dads friend. All gave same replies i.e. their labs are full.

So my dad suggested me to return to college and do a project there, as something is definitely better than nothing. Just then my mom suggested that why dont you try mailing at IIT indore It was just 25 kms from the place I reside. As far as I knew IIT Indore had only CS,EE and ME in there bachelors curriculum, so there was no point finding a chemical intern there . I started inquiring from my friend who is doing his Bachelors in CS from IIT Indore. Then I came to know about the chemistry department of IIT Indore . It had almost 20 labs under chemistry department and most of the basic machines required in research including NMR, UV, Mass , and many more, It had two huge buildings which were operators of these stuffs. I started mailing the professors of IIT indore. And I was really astonished to see four positive replies out of 7 mails I did. I joined under the professor who called me just the next day as I had only one and a half month left with me I wanted to utilise each second left with me doing something which was really productive in future. I mailed on 28th May and joined his lab at 1st July. I later on came to know that my guide already knew my Dads friend as he gave many lectures at IIT Indore in various seminars organized each month. I was the first CST BTech to join as an intern at IIT Indore so the rules were quite liberal for me. Overall it was a great experience as my work was always compared with the PhDs and PostDocs working with me in the lab. This gave me more exposure too.

ThC: What are the benefits of doing such internships? Is it really necessary to apply for such internships in 2nd year itself?

Pranjali: My Parents want me to do masters after my Btech. My dad has many friends who are professors at various government or private engineering colleges of Indore. As explained by them, doing an intern in second year is beneficial because second year of Bachelor is a stage in which you are just entering your field, the field you are going to spend your life with. You are learning the ways you need to work in order to manage, sustain yourself in that field. As we already learn to handle things in the organic lab we have in our curriculum, managing things is not that tough in the research lab . The guide we are working under is also well acquainted with the fact that we are sophomores so obviously we dont possess much knowledge about the field. In my case my guide was too cooperative, As the rest of the PhDs and PostDocs who worked in the lab came by 9 in the lab, as IIT Indore had a bus at 6 for the indorians while a bus at 9 for the hostellers Sir stayed in the city while students were all hostellers. He had

ample of time for me to explain the basics of organic chemistry(He made me read jerry march in the free time he had, its the goddess of organic chemistry), ways to target useful research, writing research paper , his experiences about life when he evolved from a Btech to masters then PhD, etc. It all helps a lot.Before I joined ,even I thought that, its not necessary so why should I ? But the things I learned there were very useful. Doing an intern in second year gives you experiences which are really precious for your entire life . I would strongly recommend you all to do it , It will teach you many things which no one else might teach you yours entire life. A little patience is a must to cope with the new environment we are exposed to but the fruits of this hardship are really sweet. The other most important reason which can be considered is a recommendation, as most of the interns in third year require recommendations of two professors. If the other one is not of the home college , it might give a better impression (This thought varies from person to person).

ThC: What a trainer expect from a trainee while working on such projects? How one can cope up with it?

Pranjali: As mentioned before, the trainer is well familiarised with the fact that you are just a student of Btech second year, you dont know much about the harms of certain chemicals you are working with, you arent that responsible towards the work you are doing in comparision to the other PhDs working in the lab, you might get tensed if something wrong happens in the lab by your hands like a reaction failure, breaking of a glassware,etc. The trainee has also gone through all these stages in his life, my professor assured me each time I did a mistake that he also did this kinda one in his lab. The trainee takes care that you arent alone in lab so that lab could be handled efficiently in case of some emergency, He doesnt gives you work which require dealing with hamful chemicals. As a whole you are nurtured in a pretty assimilable way. The expectations are limited to proper attention while he/she is explaining things, being in the lab till the others are working (liberal enough to allow taking a leave in medical issues),being sincere , respecting his words, etc. These stuffs are expected by all humans we work with , so its obviously not something which is difficult to cope up with. Its very simple, If you work for a person with pure heart he/she will also in return help you in each way possible.

ThC: What is your opinion at present about the work you

did? Is it helping you to explore more in the respective field?

Pranjali: Presently I work in Ultrafast Spectroscopy Lab, under the guidance of Dr. Debabrata Seth. The field I worked in summer is completely different with the one I am working right now on. Still I feel it was beneficial to have joined catalysis lab in summers as its easier to link these two different field then, in case you are reading a paper you get many thing which belong to different fields, having a basic knowledge of all the fields is always better, you are not stuck with things often. The lab we work in have people with different ideas to work on as the way of working and the experiences differ. Horizons broaden and thinking ability sharpens.

ThC:Suggestions for juniors!

Pranjali: I would suggest all of you to apply wherever you want, I think its not the interest in the field that matters, its the ease with which you work in that field , which decides how much you will learn working in it. As you are all in second year and dont have much knowledge of the fields you will work in as an intern, I would suggest choosing a simple ambience of doing an intern, a place where you find trainees who are free enough to give time ,helping you learn better. As I shared my experiences at IIT Indore with others , I heard back theirs, I just realised that I made a great decision joining there as My guide spent hours with me explaining things , It was possible only because he didnt had much of liabilities over himself, the institute was not much sound so it didnt had many programs, seminars, etc. Which required his time, he focused on improving our skills in the best way possible as his life at IIT Indore comprised of just we 6 working in his lab. The eminent programs which take 25 to 30 Btech students sound fancy but they might not teach us the way, these limited interns teach.Keep on mailing different proffs. , Dont get disheartened by seeing replies like unavailability of space, less funds, etc. Target small, Expect less then even little things will satiate you, Expectations hurt....

ThC: Thanks a lot for your time and all the best for future