



The Crucible

The Chemical Society
Department of Chemistry

University of Sri
Jayewardenepura

Gangodawila

Nugegoda

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EDITORIAL

Chemistry is noble and it is the key to solving many of the earth's problems. The year 2011 being the International Year of Chemistry (IYC), celebrates the achievements of chemistry and its contributions to the well-being of humankind. According to IYC, chemistry meets the global challenges of clean air, safe water, healthy food, dependable medicine, advanced materials, eco-friendly products and sustainable energy, under the unifying theme of *Chemistry-our life, our future*.

So, as chemists - as chemistry learning students - as chemistry loving people we should determine to make use of the knowledge of chemistry for the benefit of every being. Here we should extend our hearty thanks to the myriad chemists and teachers whose time, energy and expertise contribute so much to help the public, recognize the importance of chemistry.

In chemical studies one of the most valued things is discovering what no one else has discovered before. We call the process of achieving such goals as "Research". The other is the process of teaching that helps others to learn the subject. Both these are undertaken at the Department of Chemistry, University of Sri Jayewardenepura. This institution takes pride in producing persons with sound knowledge of chemistry that is immensely beneficial to the society.

Hence, it is with greatest pleasure that we present to you the eleventh issue of the publication "Crucible" as one of the many contributions from the University of Sri Jayewardenepura, to widen the chemical education at all levels.

On behalf of the chemical society, I thank all who extended their support to make the publication of this year's "Crucible", a reality.

R.H.A.C.U. Ranasinghe
(Editor)

MESSAGE FROM THE DEAN, FACULTY OF APPLIED SCIENCES

I am extremely happy to send this message of felicitation to the Chemical Society of Sri Jayewardenepura at a time when the members of the executive committee are taking every effort to bring about the eleventh edition of the magazine “The Crucible”.

A magazine of any discipline is considered to be a modus operandi for the dissemination of knowledge of that discipline. In the last year magazine we witnessed several scientific writings from our students in the Department of Chemistry. The publication of a magazine of this nature will train them among other things how to present their ideas in a manner understandable to readers. This is an integral part of the study in every discipline. In this context, scientific writing, presentation and edition play important roles. This also forms a part of their study of the discipline. I am personally aware of the motivation and enthusiasm of our students in collective work of this nature.

I also take this opportunity to thank the Head of the Department of Chemistry and members of the academic staff especially the senior treasurer for giving the necessary guidance and encouragement to the executive committee of the Chemical Society to make this venture a success.

I wish every success to all the activities of the Chemical Society.

Professor S.S.L.W.Liyanage

B.Sc. (USJ), Ph.D. (Cardiff Wales), M.I.Chem.C., MRSC, FPRI.SL.

Dean/Faculty of Applied Sciences

University of Sri Jayewardenepura

MESSAGE FROM THE HEAD, DEPARTMENT OF CHEMISTRY

I take great pleasure in sending this message to the 11th Edition of the 'Crucible', the annual publication of the Chemical Society of the University of Sri Jayewardenepura.

The Chemical Society, over the years, has done much hard work to elevate this publication to its present high standard. Every effort should be made in the future to further improve this publication, as it is now possible to access information on the latest developments in the chemical sciences through Information Technology.

Many activities were carried out by the Chemical Society in the past year, including a very informative and beneficial visit to the Tea Research Institute, Talawakelle. The Society has provided opportunities for its members to participate in many programmes and activities to develop and strengthen their skills in leadership and creativity.

This year too the largest number of students have been enrolled for Chemistry. With the increasing membership and the dedication and commitment of the President and his team, I am confident that the Chemical Society will maintain its high standard, and aspire to be the best student society in the University.

Professor Siromi Samarasinghe
B.Sc. (Vidyodaya), M.Sc., Ph.D. (Leeds), F.I.Chem.C.
Head/Department of Chemistry
University of Sri Jayewardenepura

Department of Chemistry

Academic Staff and Their Research Interests

- ❖ 


Professor Siromi Samarasinghe (Head)
B.Sc. (Vidyodaya), M.Sc.(Leeds), Ph.D. (Leeds), F.I.Chem.C.
Research Interests: Physico Chemical properties of yam starches, Polyphenols in foods and beverages, Flavor compounds in black tea, antioxidant activity of tea flavanoids.
- ❖ 


Professor S.S.L.W. Liyanage
B.Sc. (USJ), Ph.D. (Cardiff Wales), M.I.Chem.C., MRSC, FPRI.SL.
Research Interests: Synthesis of tri-phosphamacrocycles, Improvement of quality of natural rubber latex, Detailed study on degradation pattern of polymer based products.
- ❖ 


Professor A.M. Abesekara
B.Sc. (Colombo), Ph.D. (Belfast), F.I.Chem.C., FNASSL
Research Interests: Synthetic and physical organic chemistry, Bioactive natural products, Herbal drugs.
- ❖ 


Professor S.P.Deraniyagala
B.Sc. (Colombo), Ph.D. (Dalhousie), F.I.Chem.C.
Research Interests: Determination of trace metals and non-metals in food and water, Mechanism of oxidation of organic molecules by metal ions/complexes, Development of colorimetric methods to determine Low Levels of metal ions and anions.
- ❖ 


Professor P.P.M.Jayaweera
B.Sc. (USJ), Ph.D. (Belfast), M.I.Chem.C.
Research Interests: Reaction kinetics, Corrosion and Electrochemistry, Dye sensitized nano-porous photovoltaic devices, Molecular mechanics, Dynamics and semi-empirical computational calculations, Photochemistry and photophysics of labile metal complexes, Raman, Surface enhanced Raman and excited state studies of complexes and spectroscopic studies of metal colloids, Sols and MELLFs.


- ❖ 

Professor W.D.W. Jayathilake
B.Sc. (Peradeniya), M.Sc. (Bradford, UK)
Research Interests: Chemical education, Water chemistry and technology, Photoelectrocatalysis and Solar Energy conversion, Quality assurance in Higher Education.
- ❖ 

Dr. K.C.P. Mahathanthila
B.Sc. (USJ), Ph.D. (Ottawa), F.I.Chem.C.
Research Interests: Natural products chemistry
- ❖ 

Dr. Champa D. Jayaweera
B.Sc. (USJ), Ph.D. (Belfast), M.I.Chem.C.
Research Interests: Trace metal analysis, Applications of chemical kinetics in analytical chemistry, Flow injection analysis, Determination of tetracycline residues in broiler meat.
- ❖ 

Dr. Laleen Karunanayake
B.Sc. (USJ), Ph.D. (North London)
Research Interests: Use of vegetable oils and their derivatives as additives in the polymer industry, Use of locally available tannin materials to make polymer resin.
- ❖ 

Dr. Asiri Perera
B.Sc. (Colombo), M. Sc., Ph.D. (Wichita State University)
Research Interests: Comparison of migration behavior of contaminants from plastic bottles to food, Clearance of bisnitrophenylphosphate using peptides.
- ❖ 

Dr. Nilwala Kottegoda
Ph.D. (University of Cambridge, UK)
Research Interests: Material chemistry and nanochemistry.



Dr. S.D.M.Chinthaka

B.Sc. (USJ), Ph.D. (Wayne State University, USA)

Research Interests: Metal ion affinities of commonly used MALDI matrices determined by Guided ion beam Tandem mass spectrometry, Implication for MALDI mass analyses, Determination of trace levels of organic pollutant in environment by solid phase micro extraction (SPME) coupled with GC and GC-MS, Dispersive liquid-liquid extraction (DLLM) of organic pollutant in surface water, Pre-concentration and analysis of organic and inorganic pollutants by cloud point extraction (CPE) coupled with AAS, GC and GC-MS.



Dr. Chayanika Padumadasa

B.Sc. (Colombo), Ph.D. (University of Oxford, UK)

Research Interests: Natural products chemistry, Synthetic organic chemistry



Dr. Theshini Perera

B.Sc. (Colombo), Ph.D. (Louisiana State University, USA)

Research Interests: Synthesis of inorganic complexes (Re, Pt, Ru) of biomedical relevance, Applications of 1D and 2D NMR and other spectroscopic methods to characterize structure and properties of metal complexes.



Dr. M.A.B.Prashantha

B.Sc. (USJ), Ph.D. (University of Moratuwa)

Research Interests: Renewable raw materials and Alkyd resins.



Dr. Mahesh Karunarathne

B.Sc. (USJ), Ph.D. (Wayne State University, USA)

Research Interests: Nano chemistry



Dr. Thilini Gunasekara

B.Sc. (Colombo), Ph.D. (Bowling Green Ohio, USA), Industrial Post Doc. (Spectra Group Ink, OH, USA), Post Doc. (University of Texas at Austin, TX, USA)

Research Interests: Polymer synthesis and characterization, Smart polymer materials, Polymer chemistry in petroleum engineering.



Dr. Pahan Godakumbura

B.Sc. (USJ), Ph.D. (Wayne State University, Michigan, USA), Post Doc. (University of Illinois, Chicago, USA)

Research Interests: Bio-inorganic and Bio-organic chemistry, Nanoparticles in biological applications and medicine.

How soap cleans.....

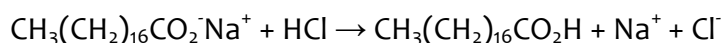
Soaps are sodium or potassium fatty acids salts, produced from the hydrolysis of fats in a chemical reaction called saponification. Each soap molecule has a long hydrocarbon chain, sometimes called its 'tail', with a carboxylate 'head'. In water, the sodium or potassium ions float free, leaving a negatively-charged head.

Soap is an excellent cleanser because of its ability to act as an emulsifying agent. An emulsifier is capable of dispersing one liquid into another immiscible liquid. This means that while oil (which attracts dirt) doesn't naturally mix with water, soap can suspend oil/dirt in such a way that it can be removed.

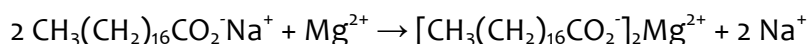
The organic part of a natural soap is a negatively-charged, polar molecule. Its hydrophilic (water-loving) carboxylate group ($-\text{CO}_2^-$) interacts with water molecules via ion-dipole interactions and hydrogen bonding. The hydrophobic (water-fearing) part of a soap molecule, its long, nonpolar hydrocarbon chain, does not interact with water molecules. The hydrocarbon chains are attracted to each other by dispersion forces and cluster together, forming structures called *micelles*. In these micelles, the carboxylate groups form a negatively-charged spherical surface, with the hydrocarbon chains inside the sphere. Because they are negatively charged, soap micelles repel each other and remain dispersed in water.

Grease and oil are nonpolar and insoluble in water. When soap and soiling oils are mixed, the nonpolar hydrocarbon portion of the micelles break up the nonpolar oil molecules. A different type of micelle then forms, with nonpolar soiling molecules in the center. Thus, grease and oil and the 'dirt' attached to them are caught inside the micelle and can be rinsed away.

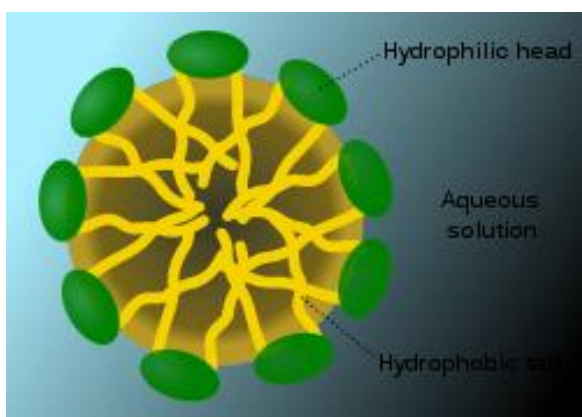
Although soaps are excellent cleansers, they do have disadvantages. As salts of weak acids, they are converted by mineral acids into free fatty acids:



These fatty acids are less soluble than the sodium or potassium salts and form a precipitate or soap scum. Because of this, soaps are ineffective in acidic water. Also, soaps form insoluble salts in hard water, such as water containing magnesium, calcium, or iron.



The insoluble salts form bathtub rings, leave films that reduce hair luster, and gray/roughen textiles after repeated washings. Synthetic detergents, however, may be soluble in both acidic and alkaline solutions and don't form insoluble precipitates in hard water.



A soap micelle has a hydrophilic head that is in contact with the water and a center of hydrophobic tails, which can be used to isolate grime.

N.S. Suwandaratne
Chemistry special 3rd year ('10/'11)

Ode To A Proton

Oh proton, how your positive charge makes me blush!
I watch you from a distance, and my heart just turns to mush...
If only I was a neutron, we could frolic for awhile,
and then my dear I'm sure, I would wear a permanent smile.
But alas, I'm an electron, and I must watch you from afar,
so far from where you are.

It seems to me that my fate is sealed,
but how can my love not be revealed?
My mass will not be complete until you are mine,
so give me this chance, and show me a sign.
Some day our gazes will meet, and I'll see your eyes,
and we will meet together and neutralize...
so until that day, farewell my opposite attract,
my love for you will always stay intact.

Nano in textiles and clothing

Nano style

Nano is used in textiles mainly to provide stain-resistance or anti-bacterial properties. Some clothes made from these textiles can now be purchased in high-street shops, usually with these properties described on the tags attached, though they may not mention the words nano or nanotechnologies.

Stain-resistant fabrics

If you spill something, even something as drastic as red wine, down the front of your nano-enhanced shirt or suit, all you have to do is wipe it off with a dry cloth and it looks like new. This is often called The Lotus Effect

What is the 'Lotus Effect'?

The leaves of a lotus plant actually repel water and other liquids, even glues. They are structured so that when it rains, little beads of water form on the plant's leaves and instead of spreading out, they just roll off.

The plant does this using its own nanotechnology. Basically, nano-sized hairs combine with the wax coating of the leaf to make the water droplets sit up on the surface without dispersing onto the leaf's surface below.

This doesn't just happen with lotus leaves. A similar process works for some insects, the wings of butterflies and the proverbial 'water off a duck's back'. Whenever a textile, or other product like glass or paint, repels water in this way, it is referred to as the Lotus Effect.

The 'Lotus Effect' in fabrics

Nano coatings (such as Teflon-like substances) are created and bond with the textile, so that little nano-sized molecular hooks attach to the fabric of the garment and the hair-like structures repel the water like the lotus leaf. But because these are nano-sized they don't make the fabric stiff, so keeping the softness of whatever is coated.



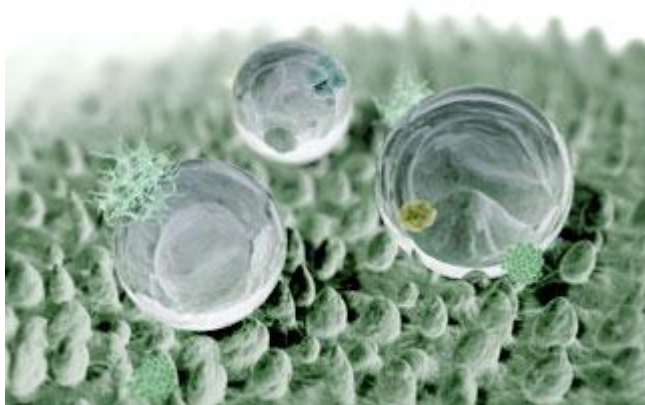
The 'Lotus Effect' in fabrics

Anti-bacterial fabrics

Silver nanoparticles are being included in a lot of different fabrics as anti-bacterial agents to stop smelly socks and odorous armpits. They are also used in pillows, bedding and fabrics of other products to kill bacteria.

These silver nanoparticles are either incorporated into the fibres of the fabric, or coated on afterwards. If they are impregnated into the material then the useful effect lasts longer than if they are coated on the surface.

Goose-down jacket fillings clump up when the garment is washed, but some no longer need to be washed ever because they are anti-stain, and use the silver nanoparticles to keep them fresh.



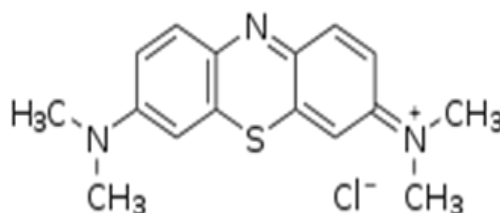
H.A.G. Hathurusinghe
Chemistry special 3rd year ('10/'11)

Two sodium atoms were walking along the street when one stops and says, "Oh my goodness, I think I've lost an electron!" "Are you sure?" asks his companion. "Yes," replies the first sodium atom. "I'm positive."

Methylene Blue as an Antimalarial Agent..!!

The first thing that comes to our mind about methylene blue is that it can be used as a redox indicator in laboratory. Basically it is a heterocyclic aromatic chemical compound which appears as an odorless, dark green solid powder in room temperature and yields a blue solution when dissolved in water. But apart from that, it has a significant value in a range of different fields such as chemistry, biology, medicine and aquaculture etc.

If the structure of methylene blue is concerned it has the basic quinoline ring which in terms responsible for antimalarial properties. Quinolines target a biological process that is totally unique to malarial parasite, i.e. *Plasmodium* sp. Among the various classes of quinolines, 8-aminoquinolines play a vital role as antimalarial agents.



The history of 8-aminoquinolines for malaria began over 100 years ago when Paul Ehrlich, the “father of chemotherapy”, observed selective uptake and staining of tissues by dyes such as methylene blue. The selectivity arises due to presence of specific receptors to which the dye can bind and that could affect the parasites residing within those tissues by targeting these receptors. Discovery of antimalarial properties of methylene blue led to the development of 8-aminoquinolines.

Though methylene blue had antimalarial properties, it was disappeared as an antimalarial drug during the Pacific War in the tropics. Apparently it was disliked by the patients because of reversible side effects: turning the skin / urine green, and the sclera (the white of the eyeballs) blue. However interest in its use as an anti-malarial has recently been revived especially due to its availability and low price. Several clinical trials are in progress, trying to find a suitable drug combination. Moreover, recent attempts have appeared more promising.

D. L. Abeyawardhane
Chemistry Special (Part 1) (‘10/’11)

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High energy in sunlight comes in two portions:

- UV-A (320–400 nanometers, or 1.2×10^{-5} – 1.6×10^{-5} inches)
- UV-B (290–320 nanometers, or 1.1×10^{-5} – 1.2×10^{-5} inches)

Since the light of shorter wavelength radiation is more energetic, UV-B causes burning, while UV-A promotes tanning. Exposure to UV-A causes eventual wrinkling and aging of the skin and these UV rays carry high energy and are suspected to cause cancer by damaging **DNA**.

A well-designed sunscreen blocks harmful ultraviolet (UV) rays and allows the skin to tan.

The most common ingredients in sunscreens are

- Zinc oxide (ZnO)
- Titanium dioxide (TiO₂)
- p-Aminobenzoic acid (PABA)
- Octylmethoxycinnamate
- Octylsalicylate

Zinc oxide (ZnO) and titanium dioxide (TiO₂)

These are long-term ingredients of most sunblockers, considered broad-spectrum agents because they block all UV light. Many sun worshipers or outdoors enthusiasts apply a coat of reflective zinc oxide and cream to their noses and ears for extra protection.

p-Aminobenzoic acid (PABA)

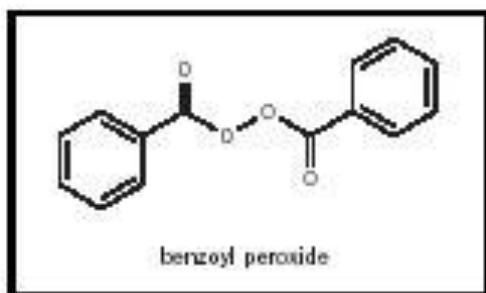
Absorbs the energy of UV-B while allowing UV-A to pass through. Other aromatic organic compounds such as benzophenone or oxybenzone are used with or in place of PABA. In the formulation process chemists must choose emollients and sunscreens that remain dispersed without precipitating from solution and feeling gritty.

Although probably harmless at the low concentrations used, most aromatic organic compounds pose some risk of cancer or of interference with bodily hormones, but this risk is probably lower than that of skin cancer or wrinkles. New technology allows encapsulation of the active ingredients of sunblockers in tiny polymer bags that keep the chemical agents away from the skin.

Dihydroxyacetone (DHA) acts as a self-tanning agent to give sunless tans. The browning action probably involves the reaction of DHA with free amino acids to form melanoidins. Melanoidins probably offer only slight UV protection.

SPF(sun-protection factor)

SPF or sun-protection factor is used to rate the Sunscreens' ability to absorb or reflect damaging wavelengths. For instance a person protected with a factor-15 sunscreen will be able to stay in the sun fifteen times longer than if unprotected. They can be classified as either UVA or UVB sunscreens depending the wavelengths they absorb. Benzophenone 4, a water-soluble UV filter, is commonly used to protect the color of cosmetic products.



Structure of Benzoyl peroxide.

Anuradhi
Chemistry special 3rd year ('10/'11)

Chemistry... is like the maid occupied with daily civilization; she is busy with fertilizers, medicines, glass, insecticides ... for she dispenses the recipes.

Jean Jacques

Chemistry: that most excellent child of intellect and art.

Sir Cyril Norman Hinshelwood

Caffeine



Caffeine is a bitter, white crystalline xanthine alkaloid that acts as a stimulant drug. Caffeine is found in varying quantities in the seeds, leaves, and fruit of some plants, where it acts as a natural pesticide that paralyzes and kills certain insects feeding on the plants. It is most commonly consumed by humans in infusions extracted from the bean of the coffee plant and the leaves of the tea bush, as well as from various foods and drinks containing products derived from the kola nut. Other sources include yerba maté, guarana berries, guayusa,

and the yaupon holly.

In humans, caffeine acts as a central nervous system stimulant, temporarily warding off drowsiness and restoring alertness. It is the world's most widely consumed psychoactive drug, but, unlike many other psychoactive substances, it is both legal and unregulated in nearly all parts of the world. Beverages containing caffeine, such as coffee, tea, soft drinks, and energy drinks, enjoy great popularity; in North America, 90% of adults consume caffeine daily.

Physical effects

- Consumption of large amounts of caffeine - usually more than 500 mg per day - especially over extended periods of time, can lead to a condition known as *caffeinism*. Caffeinism usually combines caffeine dependency with a wide range of unpleasant physical and mental conditions including nervousness, irritability, restlessness, insomnia, headaches, and heart palpitations after caffeine use
- There is little or no evidence that caffeine consumption increases the risk of cardiovascular disease, and it may somewhat reduce the risk of type 2 diabetes. There is some evidence that drinking four or more cups of coffee per day may have a minor protective effect against hypertension; however abstaining from caffeine may reduce the risks even more.
- Caffeine increases intraocular pressure in those with glaucoma but does not appear to affect normal individuals.
- It may protect people from liver cirrhosis.
- Caffeine may increase the effectiveness of some medications including ones used to treat headaches.^[23]

Caffeine consumption during pregnancy does not appear to increase the risk of congenital malformations, miscarriage or growth retardation even when consumed in moderate to high amounts. However as the data supporting this conclusion is of poor quality some suggest limiting caffeine consumption during pregnancy.

For example the UK Food Standards Agency has recommended that pregnant women should limit their caffeine intake, out of prudence, to less than 200 mg of caffeine a day-

the equivalent of two cups of instant coffee, or one and a half to two cups of fresh coffee. Although the evidence that caffeine may be harmful during pregnancy is equivocal, there is clear evidence that the hormonal changes associated with pregnancy slow the metabolic clearance of caffeine from the system, causing a given dose to have longer-lasting effects (as long as 15 hours in the third trimester).

When doses of caffeine equivalent to 2-3 cups of coffee are administered to people who have not consumed caffeine over the previous days, they produce a stimulation in urinary output. Because of this diuretic effect, some authorities have recommended that athletes or airline passengers avoid caffeine in order to reduce the risk of dehydration.

Chocolate derived from cocoa beans contains a small amount of caffeine. The weak stimulant effect of chocolate may be due to a combination of theobromine and theophylline, as well as caffeine. A typical 28-gram serving of a milk chocolate bar has about as much caffeine as a cup of decaffeinated coffee, although some dark chocolate currently in production contains as much as 160 mg per 100g

Various manufacturers market caffeine tablets, claiming that using caffeine of pharmaceutical quality improves mental alertness. These effects have been borne out by research that shows caffeine use (whether in tablet form or not) results in decreased fatigue and increased attentiveness. These tablets are commonly used by students studying for their exams and by people who work or drive for long hours. One U.S. company is also marketing dissolving caffeine strips as an alternative to energy drinks. Another unusual intake route is SpazzStick, a caffeinated lip balm.

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"A tidy laboratory means a lazy chemist."

Jöns Jacob Berzelius (Swedish chemist, 1779-1848)

Revealing Latent Fingerprints Using Ninhydrin

Ever since the early 1900's, fingerprints have been successfully used to solve crimes. The success has been accredited to fingerprints' ability to identify a suspect at the exclusion of all others. No two fingerprints have ever been found alike. In addition, during the course of one's activities, fingerprints are left on several types of surfaces. Many processing techniques have been developed allowing fingerprints to be enhanced on many of these surfaces. Each technique has the ability to selectively interact, or chemically react, with a component, or several components, found within the fingerprint residue. Fingerprints continue to be highly recognized as extremely valuable evidence

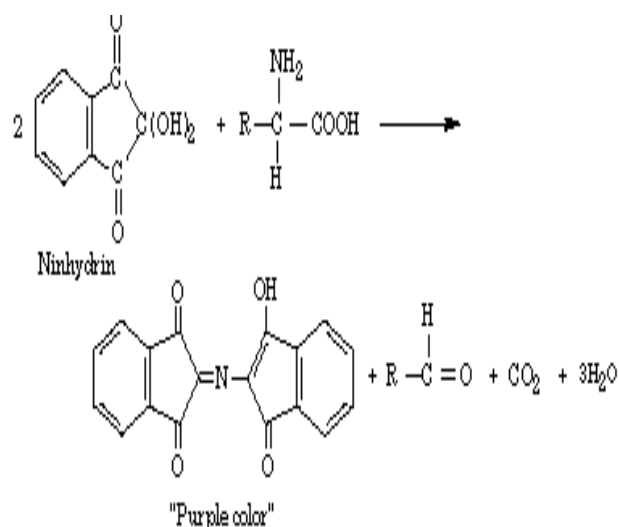


A **ninhydrin** solution is commonly used by forensic investigators in the analysis of latent fingerprints on porous surfaces such as paper. Amino acid containing fingermarks, formed by minute sweat secretions which gather on the finger's unique ridges, are treated with the ninhydrin solution which turns the amino acid finger ridge patterns purple and therefore visible.

The carbon atom of a carbonyl bears a partial positive **Ninhydrin (2, 2-Dihydroxyindane-1, 3- dione)** is a chemical used to detect ammonia or primary and secondary amines. When reacting with these free amines, a deep blue or purple color known as **Ruhemann's purple** is produced. Ninhydrin is most commonly used to

detect fingerprints, as the terminal amines of lysine residues in peptides and proteins sloughed off in fingerprints react with ninhydrin. Charge enhanced by neighboring electron withdrawing groups like carbonyl itself.

So the central carbon of a 1, 2, 3-tricarbonyl compound is much more electrophilic than one in a simple ketone. Thus indane-1,2,3-trione reacts readily with nucleophiles, including water. Whereas for most carbonyl compounds, a carbonyl form is more stable than a product of water addition (hydrate), ninhydrin forms a stable hydrate of the central carbon because of the destabilizing effect of the adjacent



carbonyl groups.

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