InfoChem

STUDENT SUPPLEMENT

ISSUE 123 JULY 2010

PHOSPHORUS FOOTPRINT

Carbon emissions, fresh-water supplies and pollution are commonly accounted for in environmental assessments of human activities. However, there are other chemical equations that must be balanced on a global scale if we are to cope with changing environmental conditions. One particularly important chemical is phosphorus, an essential nutrient in agriculture for the production of edible crops and animal feed.

PHOSPHORUS BALANCED

According to botanist John Lott of McMaster University in Canada who works with plant scientists at the University of Sydney, Australia, food security is essential for social stability. Most of the food consumed across the globe is either cereal crops – such as wheat, barley, maize, rice, soy *etc* – or legumes, such as peas and beans for example, all of which require a balanced phosphorus supply for optimal growth. But when these crops are harvested some phosphorus is removed from the soil and has to be replaced in the form of fertiliser.

Lott and his colleagues have analysed almost a decade's worth of data from United Nations' surveys for the years 1995–2003 for these crops. They looked at yearly totals of data on the production tonnage of seed and grain crops, land area used and yields measured in kilograms per hectare for Africa, Asia, Europe, North-Central America, Oceania, and South America. From the data they calculated the phosphorus footprint of agriculture based on the dry weight phosphorus content of each crop in the different regions.

Food crops need phosphorus

THINKSTOCK

The researchers found that approximately two-thirds (56–71 per cent) of elemental phosphorus is removed from the soil when seeds, grain and fleshy fruit crops are harvested. Depending on the soil type, this implies that considerable amounts of phosphorus would need to be added back to the land at potentially high costs.

IMBALANCES

Significantly, the researchers found imbalances. Asia, for example, consumes more phosphorus fertiliser in proportion to crop production than any other region but may not have access to affordable and stable supplies of fertiliser in the long term. 'This is a relevant topic in the light of the increasing global population since high-quality phosphorus reserves are diminishing and the cost of fertilisers is escalating rapidly with few options available to increase fertiliser phosphorus use efficiency', the team says.

They suggest that agriculture needs to be made more sustainable by using selective breeding or genetic modification to produce crop strains that need less phosphorus.

David Bradley

The reaction

The RSC has launched a new website, The reaction, which invites you to find out about the chemistry behind the headlines and how chemistry affects our lives. The website will also live-stream talks held at the RSC's Chemistry Centre in London and hosts videos of cool chemistry experiments. Visit www.thereaction.net to see more.

IN THIS ISSUE

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CSI: CHEMICAL SCIEN

This is the first in a short series of articles that explore the role of chemistry and chemical scientists in forensic investigations.
In this issue: Britain's biggest mass murder

On 21 December 1988 Pan Am flight 103 left Heathrow Airport bound for New York. When the Boeing 747 was 31 000 feet over Lockerbie in Scotland it dropped from the sky, killing all 259 passengers, the crew and 11 people on the ground. The devastation was made worse by 91 tonnes of fuel exploding when one of the fuel tanks hit the ground. But what was originally thought to be a tragic air accident turned out to be Britain's biggest mass murder. How was this conclusion reached?

Initial evidence

As is usually the case, the forensic investigators began with a visual inspection of the scene before collecting any samples for future analyses. This was not straightforward at Lockerbie, there were human remains and aircraft fragments spread over 845 square miles. Significantly, they found one piece of metal that was torn and twisted in such a way that only an explosive device could have caused the damage. On recovery, the flight recorder confirmed that everything was working correctly immediately before the plane disintegrated.

The metal fragment was identified as part of the forward luggage compartment, so the investigators looked for other debris that indicated close proximity to the source of the explosion. They found bits of a Samsonite suitcase, a blue Babygro (Primark) and fragments from a Toshiba radio-cassette player.

Eventually, tens of thousands of parts were collected, which enabled most of the Boeing 747 to be painstakingly reconstructed in an aircraft hanger in Farnborough. The forensic investigation, which in the main involved chemical analyses and detailed visual

Capturing visual evidence

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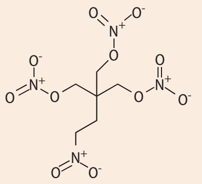
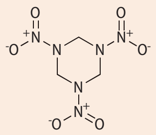
NTISTS INVESTIGATE



(*1*) Pentaerythritol tetranitrate, PETN



(*2*) Cyclotrimethylene trinitramine(RDX)

inspection of the debris, was done by scientists at the Royal Armaments R&D Establishment at Fort Halsted in Kent.

Chemical analysis

Chemists focused on the surface of the twisted metal fragment, which was pitted and blackened. Blackening is produced by un-burnt carbon from explosive organic compounds; pitting is associated with small hot particles being blasted into the metal surface.

By using capillary gas chromatography (GC), they were able to detect and identify explosive residues – *ie* volatile organic compounds – on the metal. They collected a sample for analysis by wiping the surface with cotton wool moistened with solvent, such as acetone (propanone), and injected an extract (*ca* one microlitre) from this into the heating chamber of the gas chromatograph, where it evaporates. The vapour produced mixes with a flow of helium (the carrier gas), which carries the sample vapour to a coiled capillary tube (the column). This tube is coated on the inside with a wax (usually a silicone wax) and is maintained at an elevated temperature inside a precision oven. In the vapour mixture the molecules experience forces of attraction with the wax. Different molecules are attracted to different extents, causing the molecules to become separated as they flow through the capillary tube.

As the separated molecules emerge from the capillary tube they are carried to a detector that produces an electrical signal. Finally, the signal goes to a computer attached to a chart recorder and produces the chromatogram that shows a set of peaks, with each peak corresponding to a particular compound. In the case of organic explosives, quite often a particular explosive can be recognised, not only by the main peaks, but also by peaks from traces of reactants and other compounds used in the manufacture of the explosive or formed during the explosive reaction.

By comparing the chromatograms with those obtained from standard compounds, the chemists concluded that the surface resides from the metal fragment clearly showed the presence of PETN, pentaerythritol tetranitrate (*1*) and RDX, cyclotrimethylenetrinitramine (*2*). It is common for traces of unexploded material to remain after the blast and become impacted into surrounding materials, and other compounds detected confirmed that the explosive was Semtex H, a plastic explosive manufactured in the Czech Republic. Calculations showed that the mass of explosive was around 400 g.

Crime stoppers...

Vital evidence

In cases where materials are torn apart scientists will inspect the fragments visually, possibly using the microscope or even a hand lens. Fibrous materials, in particular, provide useful information. In the Lockerbie case, scientists examined fibres from the blue babygro as well as fragments from the splintered edges of the Samsonite suitcase, both of which provided vital

Pan Am 103 reconstructed

COLIN CUTHBERT/SCIENCE PHOTO LIBRARY; REUTERS/CORBIS

"...AN IMPROVISED EXPLOSIVE DEVICE WAS IN THE SUITCASE..."

In memory...

information in reaching the final conclusions.

Visual examinations revealed that a radio-cassette player had been packed into the Samsonite suitcase surrounded by clothing and that the explosive was contained within the radio-cassette player. Blue and white fibres were found mixed with fragments of paper that were identified as coming from the owner's manual for the Toshiba radio-cassette player.

Clothing labels from fragments of material, showing close-range blast damage, suggested a Maltese connection and it was not long before police had traced the shop that supplied the clothes. The assistant handling the sale was to become a key witness because he remembered that it was a man of Libyan appearance who had bought the clothes. The assistant's memory was especially clear because he remembered the customer's behaviour was not quite normal. A picture was beginning to emerge from the jig-saw of hundreds of thousands of bits of information.

Case closed

The forensic evidence supported the theory that an improvised explosive device (IED) was in the suitcase when it was placed into the cargo hold. The bomb, activated by an electronic timer, exploded when the aircraft was over the Lockerbie area, causing a 20-inch diameter starburst hole in the aircraft's skin. Flying at almost 500 mph, the airstream stripped off the panels and caused catastrophic damage to vital hydraulic and electrical equipment that threw the aircraft out of control. From then on the aircraft disintegrated.

As in many forensic cases chemical analysis played a vital role in solving it. In this case the culprit was found, convicted of murder and a sentence of 27 years imprisonment imposed.

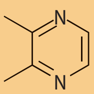
Tony Hargreaves

that's chemistry

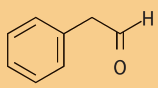
Simon Cotton looks at the molecules in our lives. In this issue: **chocolate**

Why does chocolate taste so good?

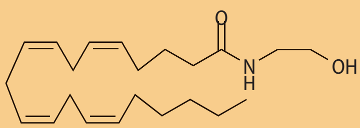
First, chocolate melts in your mouth because its melting point is *ca* 34 °C, which is just below body temperature, and so it cools the mouth. The taste of chocolate, however, comes down to a blend of around 300 flavour compounds. Chemists have identified the dominant flavour molecules as substituted pyrazines, which are aromatic compounds of the formula $C_4H_{4-n}R_nN_2$ (where R = an alkyl group). They are produced when sugars and amino acids react during roasting of the cocoa beans.



(*1*) 2,3-Dimethylpyrazine



(*2*) Phenylethanal



(*3*) Anandamide

STEFAN ZACKLIN/EPA/CORBIS; THINKSTOCK

Pyrazines with a couple of methyl substituents, such as 2,3-dimethylpyrazine (*1*), have a nutty odour, while trimethylpyrazines and tetramethylpyrazines have more of a cocoa and coffee smell, respectively. Aldehydes also play a significant role in the taste of chocolate – notably 2- and 3-methyl-butanal (malt/chocolate odour) and phenylethanal (*2*) (honey odour) have been identified.

What other molecules have been identified in chocolate?

Several stimulant molecules have been identified in small amounts in chocolate, such as caffeine and phenylethylamine (PEA). It is unlikely, though, that PEA ingested from eating chocolate would reach the brain.

In 1996, scientists reported that samples of cocoa powder and chocolate contained very small amounts of anandamide (*3*). This molecule binds to cannabinoid receptors in the brain, producing similar effects to cannabinoid drugs, the major components of cannabis. Depending on the source and concentrations used, cannabis can act as a stimulant, depressant or hallucinogen. However, the amounts of anandamide in chocolate are unlikely to produce these effects.

But is chocolate good for you?

Chocolate also contains substantial amounts of polyphenols, *eg* flavonols, with dark chocolate containing more than milk chocolate. Being antioxidants, flavonols will react with and remove free radicals which are involved in the the ageing process and in the progress of illnesses such as cancer and heart disease. It is interesting that Switzerland, the nation with the highest per capita consumption of chocolate, has one of the lowest levels of obesity and heart disease in Western Europe. However, more research needs to be done before doctors can recommend eating dark chocolate on a regular basis as a way of reducing heart disease.

ON-SCREEN CHEMISTRY

Jonathan Hare asks...

HOUSE PARTY: *could you float a house with helium balloons?*

Up – and away...

In the cartoon, *Up*,[1] 78-year old Carl Fredicksen is about to be taken away by social services to a rather depressing old folks' home but he escapes by attaching thousands of helium balloons to his house and floating away. Could you do this in real life?

Amazing as it sounds, in July 2007, Fox News in the US reported that 'gas station owner' Kent Couch tied 105 very large helium balloons to a chair and took to the skies for nine hours, flying 193 miles.[2] According to the news report, Couch was the latest American to emulate Larry Walters who, in 1982, rose three miles above Los Angeles in a chair lifted by helium balloons. So, on a small scale it looks feasible but how many helium balloons would you need to pick up a house?

Helium is far less dense than air which is why a He balloon rises, the difference in density ($\Delta\rho$) gives us the lift:

ρ(dry air) = 1.28 kg m^{-3} = 1.28 g l^{-1}

ρ(He) = 0.18 kg m^{-3} = 0.18 g l^{-1}

So $\Delta\rho = 1.28 - 0.18 = 1.10$, *ie* about 1 g of lift for each litre of He. For a standard (30 cm diameter) party balloon which holds *ca* 15 litres this amounts to roughly 10 g of lift once you take the weight of the balloon (*ca* 5 g) into consideration. So a 50 kg person would need about 50 000/10 = 5000 party balloons to start to float!

American houses are often made of wood rather than brick. A typical three-bedroom wooden house shown in the cartoon would weigh 10 000–25 000 kg.[3] Since each helium balloon creates about 10 g of lift you would need at least 10 000 000/10 balloons – *ie* about a million balloons to lift the house!

In the film we see an enormous collection of balloons above the house, perhaps 10 times the volume of the house. If the house is 5 m × 5 m × 6 m = 150 m^3 in volume this gives us a He balloon volume estimate of 10 × 150 = 1500 m^3 = 1 500 000 litres, which would mean in the cartoon there would need to be about 1 500 000/15, *ie* about 100 000 balloons above the house. This is about a 1/10th of what would be required.

So, according to our simple calculations the thousands of balloons we see in the cartoon would be enough to lift a large garden shed but not, unfortunately, enough to lift a full-sized house...

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1. *Up*, Disney, Pixar Animation Studios, 2009.
2. Fox news story: http://www.foxnews.com/printer_friendly_story/0,3566,288809,00.html
3. http://www.infra.kth.se/fms/utbildning/lca/project%20reports/Group%206%20-%20House.pdf

Dr Jonathan Hare, The CSC Centre, chemistry department, University of Sussex, Brighton BN1 9ET (www.creative-science.org.uk/TV.html).

magnificent molecules

***Laura Howes, assistant editor, highlights her favourite molecules. In this issue:* nylon-6,6**

AFP/GETTY IMAGES/THINKSTOCK

Nylon-6,6 is an amazing molecule. Discovered by Wallace Carothers and his team at DuPont, US, in 1938, it was the world's first synthetic polymer to be produced commercially and laid the foundation of the synthetic fibre industry.

The polymer is made up of repeating units of 1,6-diaminohexane and hexane-1,6-dioic acid linked by amide bonds (–NHCO–). It is unreactive and has a high melting point (265 °C), so very resistant to heat. Drawing the polymer into thin fibres makes it strong because the polymer chains straighten, align and hydrogen bond to each other. Nylon-6,6 can be made to into bristles (for toothbrushes), or sheets to be manufactured into yarn, textiles, and cordage, and it can also be formed into moulded products.

In World War II nylon-6,6 was used to replace expensive Japanese silk to make parachutes, and for ropes and tires – and for ladies stockings. Nylon is still used today in seatbelts and flak jackets.

BACKYARD CHEMISTRY

DR HAL SOSABOWSKI PRESENTS EXPERIMENTS YOU CAN DO ON YOUR OWN

IN THIS ISSUE: modelling with milk

Many types of clays, resins, plastics and glues are liquids or very soft solids but will solidify and harden when another reagent is added. The original state might be made up of monomers, single molecules which, upon addition of another reagent, link to form an infinite chain or polymer. Other substances that harden upon addition of another reagent may do so because the second reagent causes the first to become insoluble. In this experiment the soluble protein in milk – casein – will be rendered insoluble by adding acid in the form of vinegar.

Materials

You will need:

- half a litre/one pint of milk;
- a saucepan, a sieve, and a mixing spoon;
- white wine vinegar (20 cm^3);
- laboratory gloves (or Marigold-type rubber gloves); safety glasses;
- water.

Method

Pour the milk into the saucepan and heat until it simmers. Do not allow it to boil. Add the white wine vinegar carefully as the milk simmers. As you add the vinegar you may notice that white rubbery lumps begin to form – the milk is curdling. The milk will turn less cloudy and eventually clear. You now have a saucepan full of 'curds and whey', which is largely what cottage cheese consists of. Turn off the heat and allow to cool. Sieve the solid from the liquid, which can be discarded down the sink.

With gloves on you can handle the solid – the lumps will feel rubbery and soft, not unlike Mozzarella cheese (which is formed by a similar process). The lumps can be modelled into shapes in the same way you would use Plasticine, and once you are happy with the shape this can be left to dry. After a few days, the 'milk' models will be hard, not unlike solid Parmesan cheese, which, is also formed by a similar process. The shapes you have made will be hard and can be painted.

The science

The soft lumps that form when the vinegar is added to the hot milk are casein, a protein which is soluble at pH 7 (neutral) and exists in milk as the calcium salt. Casein is insoluble below pH 4.6 (acid) and the vinegar, which is a dilute solution of acetic (ethanoic) acid, makes the milk acidic enough to precipitate out the casein, leaving the vinegar as calcium acetate (ethanoate). Casein has a high molecular mass (19 000–24 000 depending on which structure it takes) and exists as long chains, a bit like the polymers in plastics.

You can try the experiment with other acids. When I was young, I remember adding orange squash to milk. When I drank it I noticed that it had a texture (small bits of matter floating around) and it tasted slightly cheesy. The citric acid in the orange squash had caused the casein to precipitate and changed the characteristics of the milk.

Health & safety

You should wear laboratory gloves or Marigold-type rubber gloves. Boiling milk will scald.

Did you know?

The somewhat offensive smell of Parmesan cheese is caused by butyric (butanoic) acid, which can be detected by the human nose at concentrations above 10 parts per million. The same acid gives vomit its characteristic smell, and is found in rancid butter.

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TECHNOLOGY ANALYST

Ron Oren

Ron Oren has spent the past 11 months working as a technology analyst for the London Technology Network (LTN). He talks to Laura Howes about his typical day.

Ron Oren

LTN is a not-for-profit company that works to increase the cooperation between businesses and academic scientists to make UK industry more competitive. LTN started in 2001 and is owned by University College London, King's College London and Imperial College London. Technology analyst Ron is part of a team which brings together scientists in the areas of environmental technology and material science.

Technological dating agency

Ron spends about half of his time meeting and talking to scientists in academia and industry about their projects and where they could use support, and then acts as a matchmaker. Although LTN was set up to support businesses, Ron finds that academic scientists and companies are equally keen to collaborate.

Once Ron knows what his client is working on, he writes a profile of the company, detailing specific projects, which is kept anonymous to protect the client's commercial interests. The profile is uploaded onto a European database and circulated to suitable scientists on the Network. Ron will filter replies from interested scientists to select the best matches before presenting his client with a hand-picked list of potential collaborators. Once a match is found lawyers draw up a contract outlining the roles of the two parties.

The collaborations that Ron brokers can vary from one-off consultancies, through joint research programmes, to long-term partnerships between a company and a university. Ron also helps clients bid for funding, especially when the funding requires collaboration for it to be awarded. When such funding opportunities are announced, he informs scientists on the Network that he thinks may be interested and works with them to find the best partners for the project. When these collaborators apply for the funding, Ron is sometimes asked to proof-read their proposals to check mainly for typos but also for clarity.

Although his chemical knowledge is sometimes helpful, Ron thinks that it is his research experience which is most useful in his job. 'Not all of my clients are chemists but I understand what research involves and how universities work, which is important', he explains.

Networking

As well as personal introductions, Ron gets involved in organising one or two networking events a month for clients: it is his job to invite suitable people, who may or may not be part of the Network, to attend, speak and present posters.

Ron occasionally goes to external events and gives presentations about the work of the Network and the opportunities available to collaborators in the Network. Ron uses these events to make new contacts and encourage them to work with LTN.

Getting out there

Ron enjoys keeping up-to date with cutting edge research and getting out and talking to people. For him, the best moments on the job are when he hears of two of his clients making a deal or being awarded funding. ■

PATHWAY TO SUCCESS

- 2009–present, technology analyst, LTN, London
- 2005–09, PhD in polymer chemistry from the University of Cambridge
- 2004, MSc in polymer chemistry from Groningen University, The Netherlands
- 1998, Dutch, English, German, Latin, pure maths, physics, chemistry, biology at VWO level (equivalent to three A-levels), Stedelijk Gymnasium Arnhem, The Netherlands

£50 OF TOKENS TO BE WON!

Benchtalk

PRIZE WORDSEARCH No. 51

Students are invited to find the 31 words/expressions associated with batteries hidden in this grid. Words read in any direction, but are always in a straight line. Some letters may be used more than once. When all the words are found, the unused letters, read in order, will spell a further seven-letter word. Please send your answers to the Editor at the usual address to arrive no later than Tuesday 3 August. First correct answer out of the editor's hat will receive a £20 HMV token.

N	Y	R	E	T	T	A	B	D	I	C	A	D	A	E	L	R
E	L	Y	D	A	N	I	E	L	L	C	E	L	L	V	E	E
G	L	R	S	L	L	E	C	N	O	T	T	U	B	C	N	L
A	A	E	C	E	D	O	R	T	C	E	L	E	H	O	O	E
T	C	T	A	N	O	D	E	T	I	H	P	A	R	G	I	C
I	I	T	T	E	N	D	O	T	H	E	R	M	I	C	M	T
V	M	A	H	L	E	S	E	N	A	G	N	A	M	N	U	R
E	R	B	O	A	T	O	M	N	E	G	Y	X	O	I	I	O
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L	L	S	N	O	R	T	C	E	L	E	E	C	U	D	E	R
S	T	A	N	D	B	Y	B	A	T	T	E	R	I	E	S	Y

ALKALINE CELL
ANODE
ATOM
BUTTON CELLS
CATHODE
DANIELL CELL
ELECTROCHEMISTRY
ELECTRODE
ELECTROLYSIS
ELECTROLYTE
ELECTRONS
ENDOTHERMIC
EXOTHERMICALLY
GAS
GEL
GRAPHITE
LEAD ACID BATTERY
LEAK
LECLANCHE CELL
LITHIUM
LITHIUM ION
MANGANESE
NEGATIVE TERMINAL
NICAD BATTERY
NICKEL CADMIUM
OXIDATION
OXYGEN
RECHARGEABLE CELLS
REDUCE
STANDBY BATTERIES
ZINC

WORDSEARCH No. 50 winner

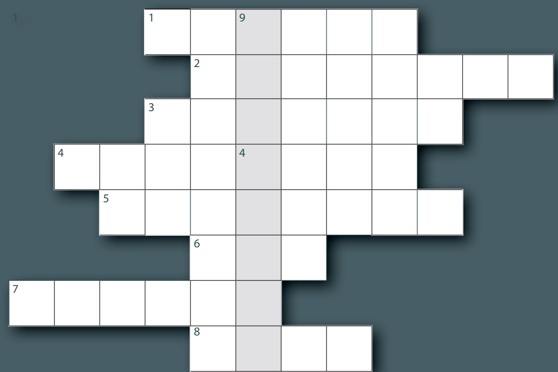
The winner was Jess Hawke from Wiltshire. The four-letter word was SALT.

FIND THE ELEMENT No. 14

Students are invited to solve Benchtalk's *Find the element* puzzle, contributed by Dr Simon Cotton. Your task is to complete the grid by identifying the eight elements using the clues below.

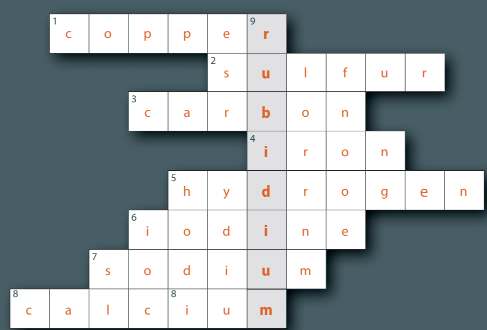
ACROSS

1. Metal used in alloy with copper to make 'silver' coins.
2. Metal used in manufacture of 'stainless steel' to stop it rusting.
3. Non-metallic element used to make semiconductors, PC 'chips' and other electronic devices.
4. When combined with nitrogen, this element forms a compound widely used in fertiliser manufacture.
5. When this element is liquified it can be used as a refrigerant for frozen foods.
6. When mixed with lead this element forms solder.
7. When mixed with acetylene gas, this element gives flame temperatures up to 3200°C.
8. Poisonous metal that was used in plumbing.



If you have completed this correctly, in 9 down you will have generated the element used in the manufacture of many disinfectants, such as Dettol, TCP and DDT. When DDT was introduced in World War II, it was such a success with the Allies that the German troops were 8000 times lousier than British soldiers. It is also an essential ingredient in PVC.

Please send you answers to: the Editor, *Education in Chemistry* the Royal Society of Chemistry, Thomas Graham House, Cambridge CB4 0WF, to arrive no later than Tuesday 3 August. First out of the editor's hat to have correctly completed the grid will receive a £30 HMV token.



Find the element no. 13 solutions and winner

The winner was Thomas Rose from Eccles Sixth Form Centre, Salford.