Two in one
The chemistry of shampoo and conditioner
Some people spend a great deal of money on various bottled potions for their hair, and new products are constantly being released. It is a highly competitive market, with much money spent on celebrity endorsements and advertising campaigns. With brands having numerous different products, have you stopped to wonder what varied bits of chemistry they contain? This ‘Lifestyle chemistry’ explores some of the chemistry behind hair shampoos and conditioners, including how chemistry can help you to have lovely shiny hair.

What is hair?

The hair on your head is made up of three main layers (Figure 1):

- The outermost layer is the cuticle. The cuticle layer has scale-like structures that cover the hair’s surface, protecting the hair strand as well as providing certain aesthetic properties, such as shine.
- The cortex lies beneath the cuticle layer and contains the pigments that provide the hair’s colour.
- The layer running through the centre of the hair strand is known as the medulla.

All three layers are made up of protein-rich dead cells. Hair freshly emerging from the hair follicles, i.e. near the scalp, has had far less exposure to sources of physical or chemical damage, such as heat from blow-drying or hair dye. These processes can damage and weaken the cuticle layer, decreasing its quality as the hair proceeds from root to tip (Figure 2).

The hair is coated in oil secreted by glands near to the hair follicle. This provides a degree of protection to the cuticle...
surface. This layer of oil is also good at absorbing any grease and dirt it is exposed to, as well as compounds contained in styling products. This means that our hair needs frequent washing to keep it feeling and looking clean. The layer of oil cannot be rinsed off with water due to its hydrophobic nature, so shampoos are used to help clean your hair.

**Soaps and surfactants**

The term ‘shampoo’ is believed to have originated from colonial India, where it referred to a head massage, often with pleasant-smelling oils. During the nineteenth century, the word came to mean the application of soap to the hair in order to clean it.

Cleansing agents like soaps and detergents are able to make oily and greasy substances more water soluble by reducing the surface tension between the two.

Soaps and detergents contain a type of molecule known as a **surfactant**. A surfactant molecule contains two parts: a hydrophilic polar head group and a hydrophobic non-polar tail group. The polar head group is attracted to other polar molecules, such as water, and repelled by non-polar molecules such as oils. Conversely, the non-polar tail is attracted to oils and repelled by polar molecules. A surfactant molecule will therefore position itself on the interface between an oil and water (Figure 3).

When a surfactant is added to water that contains some oil, the oil becomes surrounded by the surfactant, with its polar head groups pointing outwards towards the water. This forms an **emulsion**, causing small clusters of oil molecules to become more water soluble, allowing the two layers to mix and the oil and dirt to be rinsed away with water (Figure 4).

**Shampoo not soap**

Soaps are not suited to washing hair. They can cause irritation to the scalp and leave a thin film behind, making hair appear dull. Hair needs to be at a mildly acidic pH (about pH 4–5) in order to be at its strongest. At this pH all the non-covalent forces that hold the hair strand together are maintained.

Soap has a rather basic pH (approximately pH 8.5), which can disrupt some of the non-covalent interactions such as disulfide bonds, thereby weakening the hair. In fact, substances that are highly basic (pH 12 and above) destroy all the non-covalent interactions holding the hair together, causing it to dissolve completely. Continual use of soap on hair decreases the number of non-covalent interactions, thereby increasing the amount of weakening and damage.

Today, the majority of shampoos use surfactants that do not originate from soap. Many of those used today are **anionic** (i.e. negatively charged), such as sodium laurel sulfate (Figure 5).
Anionic surfactants tend to produce a large amount of foam and lather in which the residual dirt and oil from the hair can be contained before being rinsed away.

The cleansing action of the shampoo also removes the protective layer of oil that surrounds the hair. This usually needs to be replenished. Some shampoos contain agents that are able to condition the hair, but many people choose to use a separate conditioning formulation.

**Conditioners**

Stripping the hair of its oil coating can leave it tangled, looking dull and feeling dry. Using a conditioner after shampooing covers the hair in a protective material, leaving the hair softer and shinier. The coating helps fill in any damaged areas on the hair's surface where there may be ruts, making the strand smoother. Not only does this make the hair reflect light more uniformly and thereby appear more glossy, it also enables the hairs to slide past one another more easily, making them easier to comb and less likely to tangle.

There are several agents that can be used to achieve this, including silicones and cationic (i.e. positively charged) surfactants.

**Cationic surfactants**

Cationic surfactants, such as various quaternary amines (Figure 6), are able to coat the hair, as their positive charge is attracted to the electronegative surface of the hair strand. With the positive end of the surfactant molecule attracted to the hair, the non-polar end is exposed to the water when rinsed. The non-polar nature of this part of the molecule means it does not mix well with water, meaning a layer is left surrounding the hair after rinsing. The cationic charge of these surfactants also helps reduce the build-up of static electricity between the hair strands.

**Silicones**

Silicones — a family of compounds containing silicon atoms linked by oxygen atoms (Figure 7) — are frequently used in

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**Online archive (see p. 31)**

**Hair and hair products**


**Surfactants**


'I’m forever blowing colourful bubbles', *Chemistry Review*, Vol. 15, No. 4, p. 34.


'Roast beef and ashes to vegetarian shampoo', *Chemistry Review*, Vol. 12, No. 2, pp. 6–9.

**Silicones**


**Surface tension**


conditioning formulations. They are effective at lubricating strands of hair, enabling them to slide past each other easily and making them less likely to tangle and easier to comb.

The properties of the silicone can be altered by varying the chemical groups attached to the silicon atoms and the chain length. For example, dimethicone, a polymer contained within many conditioners, has two methyl groups bonded to each silicon atom (Figure 8), while others have far larger chemical groups bonded to the polymer chain.

Agents that coat the hair strands also temporarily fill in any holes within the cuticle layer, making the hair strand smoother. This helps to make the hair appear shinier, as a smoother surface is able to reflect the light more easily.

So next time you wash your hair, you will know why your hair feels different after shampooing compared to how it feels after conditioning. Now that you have a better understanding of what your hair-care products do, read the labels on the bottles to see if you can recognise some of the ingredients.

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Determining the yield of a reaction

When carrying out a synthetic reaction in the laboratory, it is usual to calculate the theoretical maximum yield of product for the reaction. We can compare this value to the actual mass of product in order to work out the percentage yield:

\[
\text{Percentage yield (\%)} = \frac{\text{Molar amount of product}}{\text{Max. molar yield from limiting reagent}} \times 100
\]

Example 1 shows a worked example of a yield calculation. Once you have followed it through, you should be able to solve Example 2.

**Example 1: preparation of copper sulfate**

For the preparation of copper(II) sulfate from copper(II) carbonate:

\[
\text{CuCO}_3 + \text{H}_2\text{SO}_4 + 5\text{H}_2\text{O} \rightarrow \text{CuSO}_4.5\text{H}_2\text{O} + \text{H}_2\text{O} + \text{CO}_2(\text{g})
\]

we react 5 g copper carbonate (assume this to be anhydrous CuCO\(_3\)) with 90 cm\(^3\) of 1 mol dm\(^{-3}\) H\(_2\)SO\(_4\), and get 9.2 g of the product, CuSO\(_4\).5H\(_2\)O.

What is the reaction yield?

To start, we can calculate the relative molecular masses and hence the molar amounts of the reagents:

Relative molecular mass of CuCO\(_3\) = 63.546 + 12.011 + (3 \times 15.9994) = 123.5552

So the molar mass of CuCO\(_3\) is 123.56 g mol\(^{-1}\):

Number of moles of CuCO\(_3\) = \(\frac{5.00\text{g}}{123.56\text{g mol}^{-1}}\) = 0.04 mol

As the volume of sulfuric acid is given in cm\(^3\), we need to convert to dm\(^3\) by dividing by 1000 (as there are 1000 cm\(^3\) in 1 dm\(^3\)).

Number of moles of H\(_2\)SO\(_4\) = 1 mol dm\(^{-3}\) \(\times\) \(\frac{90\text{cm}^3}{1000}\) = 0.09 mol

From the equation:

\[
\text{CuCO}_3 + \text{H}_2\text{SO}_4 + 5\text{H}_2\text{O} \rightarrow \text{CuSO}_4.5\text{H}_2\text{O} + \text{H}_2\text{O} + \text{CO}_2(\text{g})
\]

we can see that one mole of CuCO\(_3\) reacts with one mole of H\(_2\)SO\(_4\). We are reacting 0.04 moles of CuCO\(_3\) with 0.09 moles of H\(_2\)SO\(_4\) (Table 1), so we can see that the acid is in excess and...
So the molar mass of CuSO\textsubscript{4}.5H\textsubscript{2}O is 249.68 g mol\textsuperscript{-1}:

\[
\text{Number of moles of CuSO}_4\cdot5\text{H}_2\text{O} = \frac{9.2\text{ g}}{249.68\text{ g mol}^{-1}} = 0.037 \text{ mol}
\]

The percentage yield of the reaction is therefore:

\[
\text{Percentage yield} = \frac{\text{Actual yield of product}}{\text{Theoretical yield}} \times 100 = \frac{0.037 \text{ mol}}{0.040 \text{ mol}} \times 100 = 92.5\%
\]

**Example 2: reaction of benzaldehyde and pyrrole**

You react 1.65 cm\textsuperscript{3} benzaldehyde with 1.0 cm\textsuperscript{3} pyrrole and obtain 0.51 g of the desired product, tetraphenylporphyrin (Figure 1).

To calculate the molar amounts, you would need to look up the densities and the molar masses of the reactants, but we have done that for you (Table 2).

**Table 1**

<table>
<thead>
<tr>
<th>Reagent</th>
<th>Relative molecular mass</th>
<th>Amount used</th>
<th>Molar amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>CuCO\textsubscript{3}</td>
<td>123.55</td>
<td>5.00 g</td>
<td>0.04 mol</td>
</tr>
<tr>
<td>H\textsubscript{2}SO\textsubscript{4}, 1 mol dm\textsuperscript{-3}</td>
<td>90 cm\textsuperscript{3} = 0.09 dm\textsuperscript{3}</td>
<td>0.09 mol</td>
<td></td>
</tr>
</tbody>
</table>

the CuCO\textsubscript{3} is the limiting reagent. The maximum theoretical yield of the reaction is therefore equal to the number of moles of CuCO\textsubscript{3}, i.e. 0.04 mol.

Now we need to calculate the relative molecular mass (M\textsubscript{r}) and the number of moles of product (CuSO\textsubscript{4}.5H\textsubscript{2}O) we have obtained:

\[
M_r \text{CuSO}_4\cdot5\text{H}_2\text{O} = 63.546 + 32.06 + (9 \times 15.9994) + (10 \times 1.008) = 249.6806
\]

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This ‘Lab page’ has been adapted from some of the trans:it science materials. The trans:it resources are designed to help students with the transition from school/college to university. You can access the materials at [www.transit.ac.uk](http://www.transit.ac.uk).
Early on in your school chemistry lessons you probably placed various metals in hydrochloric acid and observed their relative reactivities. You will have characterised magnesium as a reactive metal, effervescing vigorously and producing hydrogen as the metal forms magnesium chloride solution. Conversely, the lack of reaction between copper and hydrochloric acid will have provided evidence that copper is simply too unreactive to react with strong acids (Figure 1). Did you ever wonder why they never let you try it with nitric acid?

Copper does react with nitric acid, producing clouds of brown nitrogen(IV) oxide and a blue-green solution of aqueous copper(II) ions. Nitric acid contains H^+(aq) and NO_3^–(aq) ions. It can’t be the H^+(aq) ions in the nitric acid reacting with the copper, otherwise other acids would react the same way. But it isn’t the NO_3^–(aq) ions either, otherwise copper would react with sodium nitrate solution, and it doesn’t.

Even though we are not trying to make electrical cells, we can use electrode potentials to help us understand what is happening. Electrode potentials are a valuable tool for considering possible redox reactions and working out whether they will actually happen, because their values tell us how powerful different reagents are as oxidising agents. You should practise using them in this way.

Here are the standard electrode potentials we will need:

- 2H^+(aq) + 2e^- → H_2(g) \quad E^* = 0.00V
- Cu^{2+}(aq) + 2e^- → Cu(s) \quad E^* = +0.34V
- NO_3^–(aq) + 2H^+(aq) + e^- → NO_2(g) + H_2O(l) \quad E^* = +0.80V
- SO_4^{2−}(aq) + 4H^+(aq) + 2e^- → SO_2(aq) + 2H_2O(l) \quad E^* = +0.17V

**Why doesn’t copper react with H^+(aq) ions?**

If copper reacted with H^+(aq) ions to produce H_2(g), the copper metal would be oxidised to copper(II) ions, so the oxidation reaction we want is:

- Cu^{2+}(aq) + 2e^- → Cu(s) \quad E^* = +0.34V

**Oxidation (loss of electrons)**

If it worked, the hydrogen ions from the acid would be reduced to elemental hydrogen gas. The reduction reaction would be:

- 2H^+(aq) + 2e^- → H_2(g) \quad E^* = 0.00V

**Reduction (gain of electrons)**

The reaction is feasible if the cell potential is positive. We define cell potential as:

\[ E^\text{cell} = E^\text{reduction} - E^\text{oxidation} \]

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**Figure 1** Magnesium reacts with hydrochloric acid (left), copper (right) does not
In this case $E_{\text{cell}}^\circ = 0.00 - 0.34 = -0.34\text{V}$, so the reaction is not feasible and copper will not react with acids in general.

**Why will copper react with nitric acid?**

The NO$_3^-$ gas given off tells us that the NO$_3^-$ ions, in which nitrogen has an oxidation number of $+5$, are being reduced (acting as an oxidising agent), because in NO$_3^-$ nitrogen has an oxidation number of $+4$. This only works in the presence of H$^+$ ions, which can react with the ‘extra’ oxygen atom from the nitrate ion. During the reaction the formation of a blue-green colour in the solution tells us that copper has been oxidised to copper(ii) ions.

The oxidation reaction we want is:

\[ \text{Cu}^{2+}(aq) + 2e^- \rightarrow \text{Cu}(s) \quad E^\circ = +0.34\text{V} \]

The reduction reaction would be:

\[ \text{NO}_3^-(aq) + 2\text{H}^+(aq) + e^- \rightarrow \text{NO}_2(g) + \text{H}_2\text{O}(l) \quad E^\circ = +0.80\text{V} \]

In this case $E_{\text{cell}}^\circ = 0.80 - 0.34 = +0.46\text{V}$, so this reaction is feasible. Copper will react with nitric acid because the H$^+$ ions allow the NO$_3^-$ ions to act as an oxidising agent.

Now you know that the reaction works, you can combine the reduction and oxidation half-equations to get the overall ionic equation for the reaction. To do this you need to get the same number of electrons in each half-equation, so the reduction half-equation needs multiplying by two throughout:

\[ 2\text{NO}_3^-(aq) + 4\text{H}^+(aq) + 2e^- \rightarrow 2\text{NO}_2(g) + 2\text{H}_2\text{O}(l) \]

Now we need to turn the oxidation reaction around so that the reactants are on the left and products are on the right, as is the convention:

\[ \text{Cu}(s) \rightarrow \text{Cu}^{2+}(aq) + 2e^- \]

Finally we add the reactants together on one side of the arrow and the products together on the other side, cancelling out anything that occurs on both sides of the arrow to get the overall ionic equation:

\[ \text{Cu}(s) + 2\text{NO}_3^-(aq) + 4\text{H}^+(aq) + 2e^- \rightarrow \text{Cu}^{2+}(aq) + 2\text{NO}_2(g) + 2\text{H}_2\text{O}(l) \]

If you are worried that there are more H$^+$ ions than NO$_3^-$ ions on the left, this is because two NO$_3^-$ ions are spectator ions: present on both the left and the right side of the equation and therefore largely irrelevant. We can put them back in, although they only serve to obscure what is really reacting with what:

\[ \text{Cu}(s) + 4\text{HNO}_3(aq) \rightarrow \text{Cu(NO}_3)_2(aq) + 2\text{NO}_2(g) + 2\text{H}_2\text{O}(l) \]

**Checking a hypothesis using electrode potentials**

If NO$_3^-$ ions can be reduced to NO$_2$ when H$^+$ ions are present, it would be reasonable to suggest that SO$_4^{2-}$ ions might be reduced to SO$_2$ when H$^+$ ions are present. Perhaps copper will react with sulfuric acid too?

The oxidation reaction we want is:

\[ \text{Cu}^{2+}(aq) + 2e^- \rightarrow \text{Cu}(s) \quad E^\circ = +0.34\text{V} \]

The reduction reaction would be:

\[ \text{SO}_4^{2-}(aq) + 4\text{H}^+(aq) + 2e^- \rightarrow \text{SO}_2(aq) + 2\text{H}_2\text{O}(l) \quad E^\circ = +0.17\text{V} \]

In this case $E_{\text{cell}}^\circ = 0.17 - 0.34 = -0.17\text{V}$, so this reaction is not feasible. Copper does not react with sulfuric acid, although we should be aware that a prediction based on standard electrode potentials assumes we will be doing these reactions with solution concentrations of 1.0 mol dm$^{-3}$ and at standard temperature and pressure (STP). Increasing the concentration of the sulfuric acid would shift the position of equilibrium to the right, increasing the value of $E^\circ$ and making the cell potential less negative and the reaction more feasible.

So now you have the tools to propose your own redox reactions and to predict whether they will work. Extensive lists of standard electrode potentials are available in data books and online (for example at www.tinyurl.com/Wikipedia-SEP-Data-page). If your reactions look promising, why not ask if you can try them out in the lab.

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**Glossary**

**Electrode potential** The potential, measured relative to some stated electrode, formed between a metal and a solution of its ions or between ions of the same element in different oxidation states. The standard electrode potential ($E^\circ$) is the potential difference between a half-cell and a standard hydrogen half-cell.

**Oxidation number (oxidation state)** A measure of the extent of oxidation of a compound, i.e. how electron deficient it is. Complexes of transition metal elements are often able to have a range of oxidation states. The oxidation number is the difference between the number of electrons associated with an element in a compound and the element itself.

**Oxidising agent** A chemical species that receives an electron (or electrons) during a reaction (becoming reduced), thereby oxidising the species that donates the electrons.

**Redox reaction** Oxidation-reduction reaction where electrons are lost by one species (oxidation) and gained by another species (reduction).

**Standard temperature and pressure (STP)** 273.15 K (0°C) and 101 325 Pa (1 atm).