

Chemistry

NOW

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The leaflets are:

•Chemistry and sport

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•Combinatorial chemistry

This is also aimed at the post-16 age group. Combinatorial chemistry is a group of techniques for synthesising large arrays of related chemicals. These can be easily automated by the use of robot syringes controlled by computers to carry out repetitive processes. The resulting arrays of chemicals called 'libraries' can then be screened for potential drug activities. Combinatorial chemistry is increasingly being used by pharmaceutical companies in their search for new drugs.

*Electron distribution
of cinnamamide*

Answers

For the use of teachers, answers to the questions on the leaflets are presented overleaf.

Chemistry and sport

One of the most amazing things about athletics is how World records continue to tumble – performances keep getting better. For example, the World record for the 100 m sprint is 9.79 seconds set by Maurice Greene in June 1999, and the Olympic record – set by Donovan Bailey at the 1996 Olympic Games in Atlanta – is 9.84 seconds. This is over two seconds better than the time of 12 seconds run in the 1896 Games – an improvement of about 20 per cent.

Chemists have contributed to these improvements in a number of ways. For example, the design of improved materials for clothing and equipment – eg poles for



▲
Donovan Bailey
setting the 1996
Olympic 100m
sprint record

FASTER AND FASTER

Performances in athletics events have steadily improved over the past 100 years as exemplified by the winning times in the Olympic men's 100 m sprint finals.

1896	Thomas Burke (US)	12.0 s
1900	Francis Jarvis (US)	11.0 s
1904	Archie Hahn (US)	11.0 s
1906	Archie Hahn (US)	11.2 s
1908	Reginald Walker (S Africa)	10.8 s
1912	Ralph Craig (US)	10.8 s
1920	Charles Paddock (US)	10.8 s
1924	Harold Abrahams (UK)	10.6 s
1928	Percy Williams (Canada)	10.8 s
1932	Eddie Tolan (US)	10.38 s
1936	Jesse Owens (US)	10.3 s
1948	Harrison Dillard (US)	10.3 s
1952	Lindy Remigino (US)	10.79 s
1956	Bobby Morrow (US)	10.62 s
1960	Armin Hary (FRG*)	10.32 s
1964	Robert Hayes (US)	10.06 s
1968	James Hines (US)	9.95 s
1972	Valeriy Borzov (USSR)	10.14 s
1976	Hasely Crawford (Trinidad)	10.06 s
1980	Allan Wells (UK)	10.25 s
1984	Carl Lewis (US)	9.99 s
1988	Carl Lewis (US)	9.92 s
1992	Linford Christie (UK)	9.96 s
1996	Donovan Bailey (Canada)	9.84 s

* FGR stands for the former Federal Republic of Germany.

Of course this list will soon be out of date. The internet is a good place to check up on changing information and one place to start with athletics records is

<http://www.hkkk.fi/~niininen/athl.html>

vaulting, spikes for running and even the track itself. Chemists are also involved in devising and monitoring the best methods of training for particular sports.

One example of this is the development of a performance test called the blood lactate threshold which helps endurance athletes – such as marathon runners – to train and prepare for competition and even helps them monitor their performance during an event.

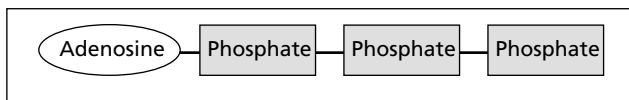
- Q1. What other factors will affect athletic improvement as well as biochemical ones
- Q2. Why is there not a steady increase in performance year on year?
- Q3. Try plotting a graph of the winning Olympic times against the year.
- Q4. Suggest why some of the times are recorded to one decimal place and others to two.

●The muscles' energy systems

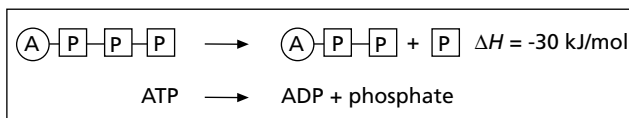
To understand the blood lactate test, we need to know something about the chemistry of how our bodies convert the chemical energy in our foods into mechanical energy, which makes our muscles contract.

The energy required for muscle contraction comes from a molecule called adenosine triphosphate (ATP, Fig 1).

In ATP, an organic (carbon-based) group called adenosine is attached to three



▲ **Figure 1**
An ATP molecule
phosphate groups. The phosphate groups are involved in the energy storage. The loss of one of the phosphate groups produces adenosine diphosphate (ADP) and gives out 30 kJ/mol of energy (Fig 2). This reaction



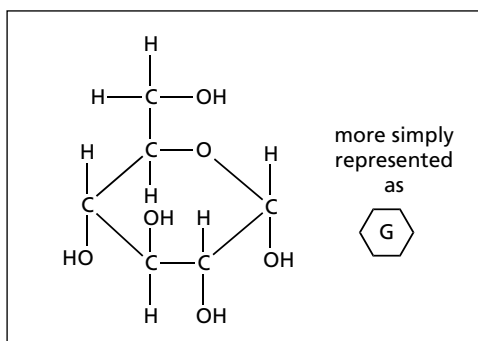
▲ **Figure 2**
The loss of a phosphate group from ATP
supplies the energy used to make our muscles contract. Surprisingly, we have only a relatively small amount of ATP in our muscles at any one time – even Olympic sprinters have enough for only two or three seconds of effort. So how can a sprinter complete a 10 second 100 m race, never mind a marathon runner keep going for over two hours?

The answer is that ATP is regenerated. The above reaction (Fig 2) is reversible and phosphate is re-attached to ADP to make ATP. This requires an input of 30 kJ/mol of energy. The energy for this comes from the breakdown of food molecules – carbohydrates (such as glucose, Fig 3), fats and proteins. The primary source is carbohydrates. These molecules store a great deal of energy (a mole of glucose (180 g) can release about 3000 kJ when reacted with oxygen). Our bodies release this energy gradually via the ATP/ADP cycle.

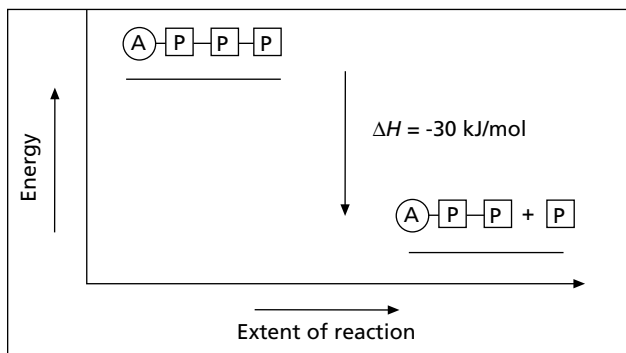
Q 5 a) What word is used to describe a reaction in which energy is; (i) given out; and (ii) taken in?

b) Figure 4 shows an energy level diagram for the formation of ADP and phosphate from ATP. Draw an energy level diagram for the regeneration of ATP from ADP and phosphate

► **Figure 3**
A glucose molecule



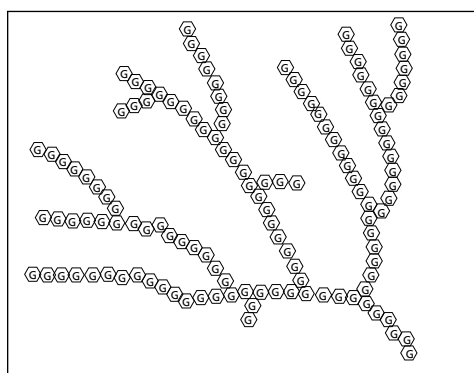
Q 6 a) How many molecules of ATP could be regenerated by one molecule of glucose if the process were 100 per cent efficient?



b) In fact the process is only 40 per cent efficient. How many ATP molecules are actually regenerated by one molecule of glucose?

▲ **Figure 4**
Energy Level Diagram

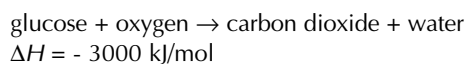
Glucose is stored in the muscles as a carbohydrate called glycogen, which consists of many glucose molecules linked together (Fig 5). Some endurance athletes make sure that they have a good supply of glycogen for an event by 'carbohydrate loading'. They eat a lot of carbohydrate (rice, pasta, bread, potatoes etc) for a few days before an event.



◀ **Figure 5**
Part of a glycogen molecule

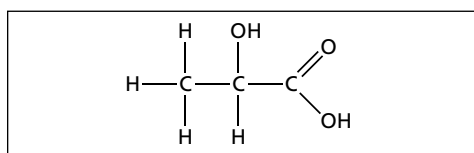
Our bodies have two ways of releasing the energy in glucose molecules – both processes are called respiration.

The first is called aerobic – 'with air' – respiration and uses oxygen to 'burn' the glucose to carbon dioxide and water



Q 7 Write the balanced symbol equation for the aerobic respiration of glucose, C₆H₁₂O₆.

The second is called anaerobic ('without air') respiration and involves splitting a glucose molecule into two molecules of lactic acid (Fig 6).

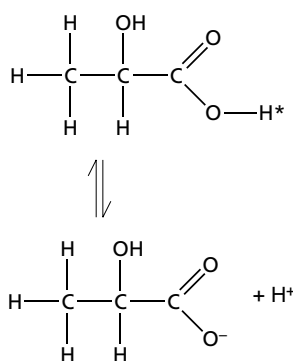


◀ **Figure 6**
Lactic acid molecule

LACTIC ACID AND LACTATE IONS

The chemical properties which we call 'acidity' (sour taste, effect on indicators, reactions with metals, carbonates hydroxides and oxides) are all caused by the H⁺(aq) ion. This is a hydrogen atom which has lost its electron so that it consists of just a proton. The substances we call acids dissociate (split up) to release this ion. In lactic acid, just one of the hydrogen atoms, the one marked * can be released to form a H⁺(aq) ion and a lactate ion.

In the body, lactic acid exists as both the acid itself and the lactate ion. For simplicity we will refer to them both as lactic acid.



Not all the molecules in a solution of lactic acid split up in this way – in fact only about four in every 100 split up in a dilute solution. Acids in which only a small percentage of the molecules are dissociated are called **weak acids**. This is in contrast with **strong acids** where all of the molecules in a solution are split up to release H⁺(aq). A good example is hydrochloric acid; in a solution of this acid, no H-Cl molecules remain undissociated.

Anaerobic respiration releases less energy than aerobic respiration.



Q 8 Glucose has the molecular formula C₆H₁₂O₆. What is the molecular formula of lactic acid? What other product is there (if any) of the anaerobic respiration of glucose?

Aerobic respiration is our main source of energy supply. It relies on a continuous supply of oxygen being provided through the bloodstream. In short-term, high-intensity activities, such as sprinting – 'oxygen debt' activities – the bloodstream cannot supply oxygen fast enough for aerobic respiration, and the body resorts to anaerobic respiration as well. Lactic acid builds up in the muscles which may be a factor in fatigue. It then

takes around 30–40 mins for the lactic acid to be cleared from the body after a period of high intensity exercise.

Some athletes attempt to delay the onset of fatigue caused by lactic acid by so-called 'bicarb loading'. Before an event, they take large quantities of sodium hydrogencarbonate (NaHCO₃), also called bicarbonate of soda or sodium bicarbonate. This is a base. It makes the blood more alkaline and reacts with the lactic acid, clearing it from the muscles faster. Some beneficial effects have been reported, but the side effects of this practice (which is quite legal) include diarrhoea, stomach cramps, bloating and nausea - not the best conditions in which to do competitive sport!

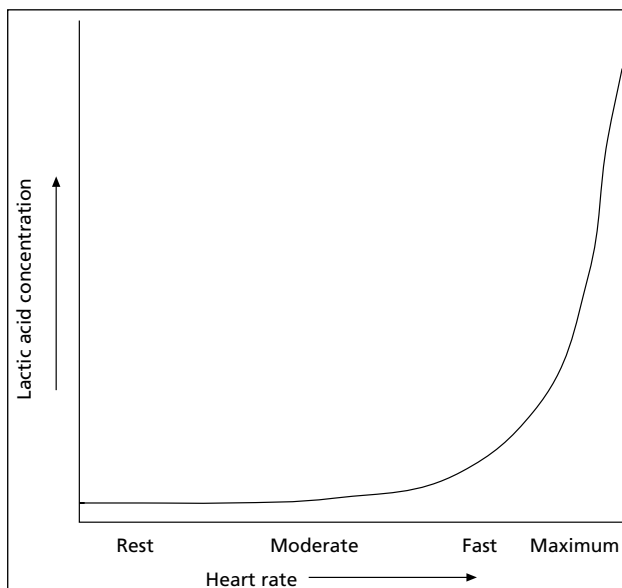
Q 9 Hydrogencarbonates and carbonates react in a similar way with acids. What gas might cause the bloated feeling in 'bicarb loading' when sodium hydrogencarbonate reacts with lactic acid?

● The blood lactate threshold

The lactic acid concentration in the blood can be measured using a test strip – rather like indicator paper – and a blood sample of no more than a single drop. The normal level of lactic acid in the blood is between 0.0045–0.09 g/dm³ but this can rise to as much as 2.25 g/dm³ after high intensity exercise such as a 400 m sprint.

Figure 7 shows a graph of lactic acid concentration in the blood against heart rate – a measure of the intensity of exercise. The **blood lactate threshold** is the heart rate at which lactic acid begins to build up in the

Figure 7
Blood lactic acid concentration
▼





blood. It is therefore the point at which anaerobic respiration kicks in. For endurance athletes, such as long distance runners, this threshold is very important. They rely on aerobic energy production to maintain their ATP level for long periods of time. If lactic acid builds up, they have moved into anaerobic energy production which can continue only for a short time. They must keep their heart rate (and therefore their exercise intensity) below this threshold to maintain their activity for a long period of time. If athletes know their blood lactate thresholds, they can keep their heart rates below them during an event. Many athletes monitor their heart rates during training and competition to do just this.

Suitable training can increase the blood lactate threshold – an untrained person's threshold is around 65 per cent of their maximum heart rate while a trained endurance athlete can achieve up to 90 per cent of their maximum heart rate.

Q10 On a copy of Fig 7; (a) mark the blood lactate threshold; and (b) sketch the graph you would expect for a trained endurance athlete.

At the moment, athletes can only measure their heart rate – not their lactic acid level – during competition. However, on-line sensors that measure lactic acid concentration in the blood directly may soon be available. These

will probably work by shining a beam of infrared radiation through the skin and through blood in the blood vessels. The radiation will be of a wavelength that is absorbed by lactic acid. The less intense the beam when it emerges, the more lactic acid there is in the blood. Such sensors might look like wrist watches. Sensors are currently being developed to measure blood glucose levels in people with diabetes, and lactic acid sensors will use similar technology.

Q 11 What is the advantage of measuring blood lactic acid levels during the race with an infra-red sensor? Are there any possible objections to this?

● Acknowledgements

This article is adapted by Ted Lister, with permission, from Mark Holmes, *On track to the Olympic games: Chemistry Giving the Winning Edge* in Australian chemistry Resource Book, Charles L. Fogliani (ed), p. 226. Queensland: Royal Australian Chemical Institute, 1998.

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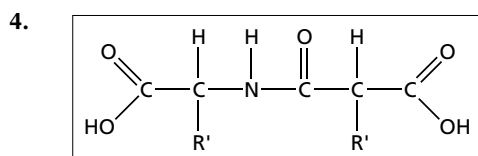
Answers

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Answers...

• Combinatorial chemistry

1. $\text{ROH} + \text{R}'\text{COCl} \rightarrow \text{R}'\text{COOR} + \text{HCl}$
2. Ethyl propanoate
3. HCl

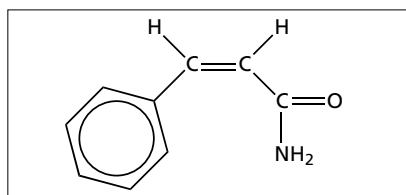


5. The corresponding tripeptide, tetrapeptide *etc.*
6. Based on A-level chemistry, students might suggest the following:
 - a) Converting the $-\text{CO}_2\text{H}$ group into an ester
 - b) Converting the $-\text{NH}_2$ group into an N-substituted amine or an amide

However, neither of the compounds in (b) is really suitable as neither is easily removable.
7. Remove water as it is formed
8. Resin-A-C, resin-B-C and resin-C-C
9. 20^4 (160 000)
10. 3.6×10^9
11.
 - a) High throughput screening for biological activity.
 - b) Robotic techniques for synthesis and sensitive analytical techniques

• Computational chemistry

1. React cinnamic acid with ammonia and then heat to dehydrate the ammonium salt produced.
2. Derivatives might include: ester, acid chloride, anhydride, salts and the parent alcohol, addition products of the double bond *etc.*
3. The $-\text{CONH}_2$ group can hydrogen bond with water but the rest of the molecule is non-polar so the solubility is not great.
4. $\text{PhCHCHCONH}_2 + \text{H}_2\text{O} \rightarrow \text{PhCHCHCOOH} + \text{NH}_3$
A nucleophilic substitution reaction.
5. a $\sim 120^\circ$, b $\sim 105^\circ$, c $\sim 121^\circ$, d = 120°
6.
 - a) This is a benzene ring and undergoes electrophilic substitution reactions.
 - b) This is an alkene and undergoes electrophilic addition reactions.
 - c) This is a carboxylic acid and undergoes acid-base reactions and nucleophilic substitution reactions
7. *trans*-3-phenylprop-2-enamide.

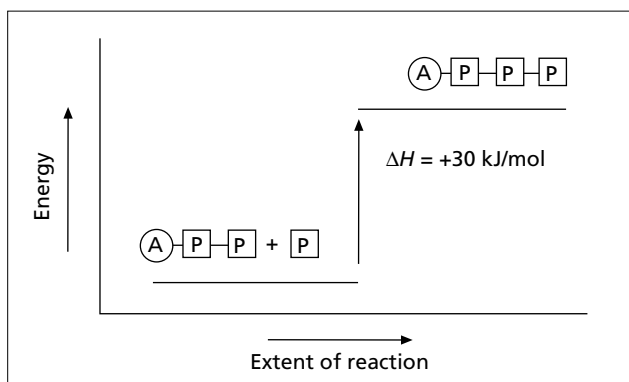


9. The C- CONH_2 bond, the C-N bond and the C-Ph bonds can rotate, the others cannot.

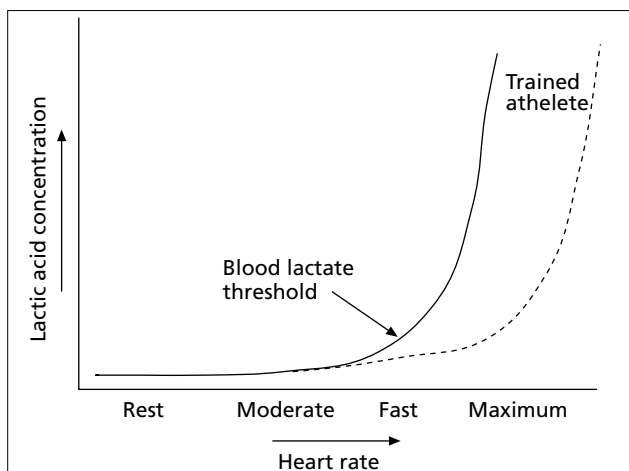
Answers...

●Chemistry and sport

- Many factors including weather, health of competitors, psychological state of competitors, equipment.
- Some of the above factors vary from competition to competition plus natural variation amongst competitors.
- Graph plotted by students.
- Improvement in timing methods from hand-operated stop-watches to electronic methods brings about greater accuracy.
- a) (i) exothermic, (ii) endothermic
b)



- a) 100
b) 40
- $\text{C}_6\text{H}_{12}\text{O}_6 + 6\text{O}_2 \rightarrow 6\text{CO}_2 + 6\text{H}_2\text{O}$
- $\text{C}_3\text{H}_6\text{O}_3$. None – all the atoms are accounted for.
- Carbon dioxide.
- Note:
The blood lactate threshold is a heart rate not a lactic acid concentration.



- Athletes will be able to respond faster to the information they get. Some athletes may not be able to afford the sensors and could be put at a disadvantage. Some might think that such reliance on technology is 'not sporting'.

Note for teachers

Lactic acid is, of course, a weak acid and at the pHs of blood and muscle it exists predominantly as lactate ions. It has not been thought appropriate to stress this point in an article aimed principally at pre-16 students. Teachers using the article with older students might wish to refer to this.

●Chemistry of the atmosphere

- a) 32, 28, 44;
b) 8, 7, 11
- There is more oxygen and nitrogen and less carbon dioxide and water vapour in the modern atmosphere.
- Fossils are the remains of once-living creatures preserved in rocks. Certain fossils are associated with certain eras.
- a) Rust
b) $4\text{FeO} + \text{O}_2 \rightarrow 2\text{Fe}_2\text{O}_3$
- Lightning might have ignited them - especially in the high level of oxygen present at the time.
- The carbon was originally in the atmosphere as carbon dioxide and was converted into carbohydrate by photosynthesis and later into coal or oil.
- Add acid and test any gas given off with limewater (aqueous calcium hydroxide). If a carbonate is present, carbon dioxide will be given off which will turn limewater milky.

●Further reading

Chemistry and sport was adapted from Mark Holmes, *On track to the Olympic games: Chemistry Giving the Winning Edge in Australian Chemistry Resource Book*, Charles L Fogliani (ed), p226, Queensland, Royal Australian Chemical Institute, 1998.

Chemistry of the atmosphere was adapted from an article by Alistair Fleming in *Teaching Earth Sciences*, 1998, 23, 130. Teachers may wish to consult the original articles for more information.

Further material on Computational Chemistry and Combinatorial Chemistry can be found in the relevant chapters of the RSC book *The Age of the Molecule* and the post-16 text based on it, *Cutting-Edge Chemistry*.