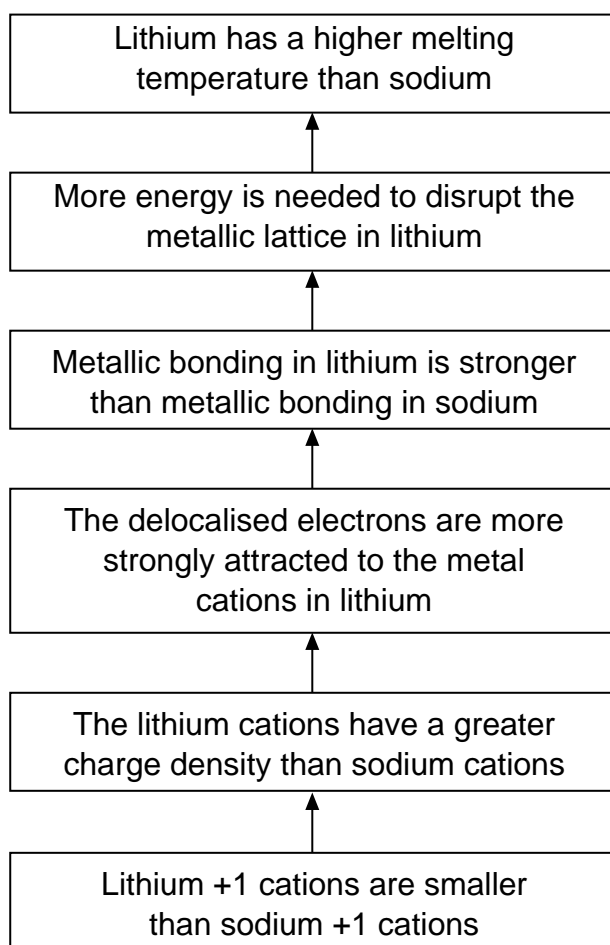


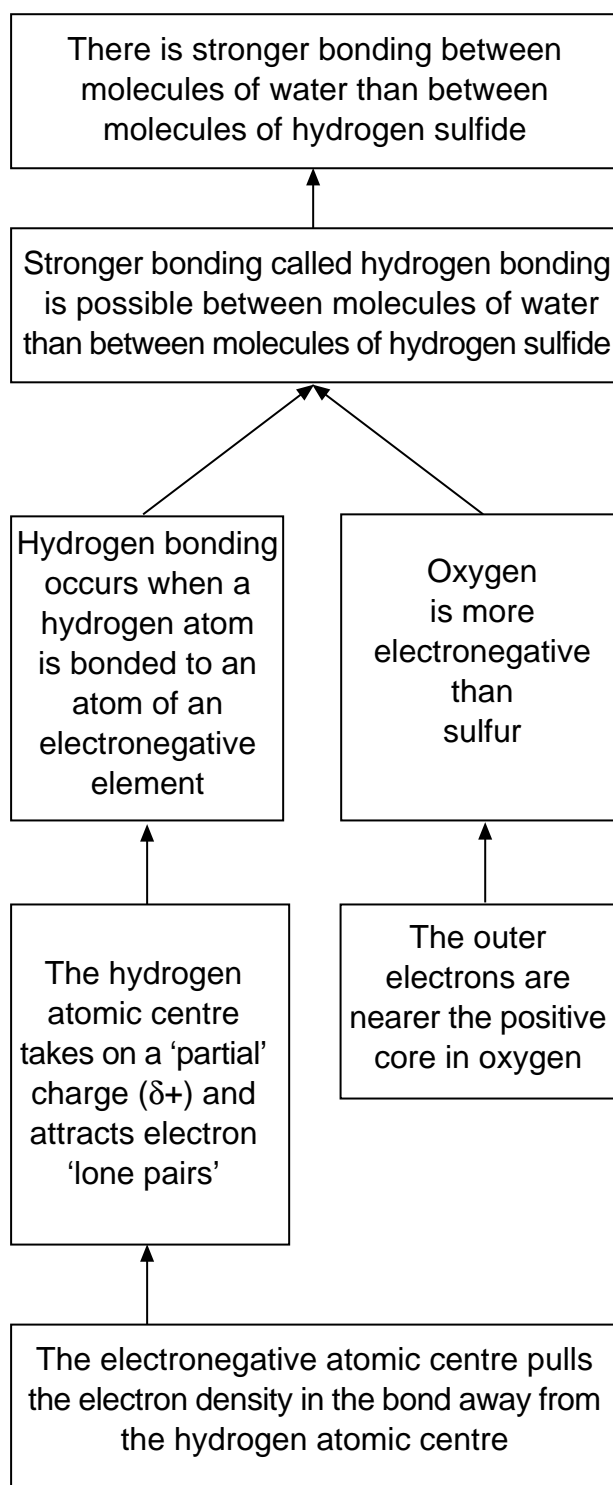
Examples of chemical explanations (1)

The following scheme may be used as the basis of explaining the eight questions included in the worksheets **Explaining chemical phenomena** (1).

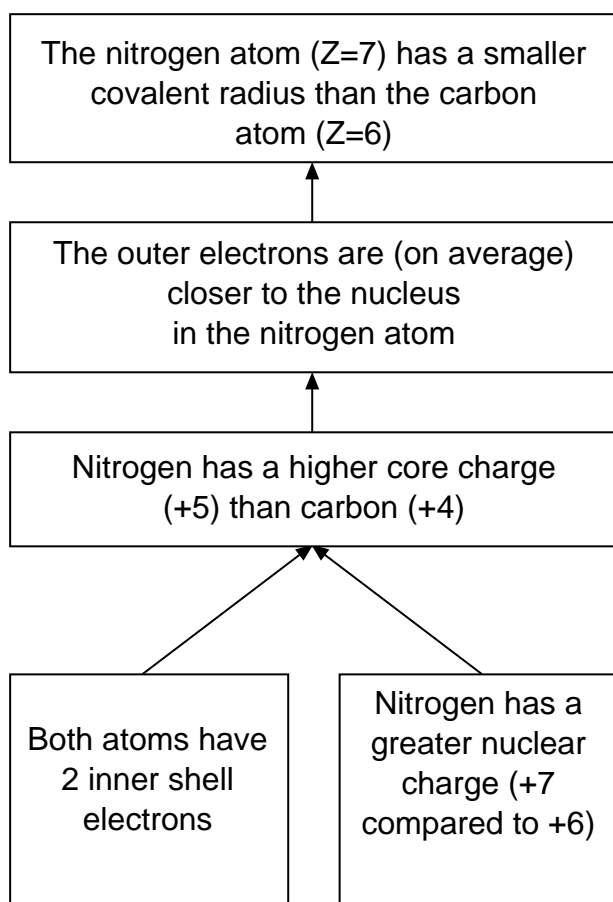
1. Lithium has a higher melting temperature (454 K) than sodium (371 K).



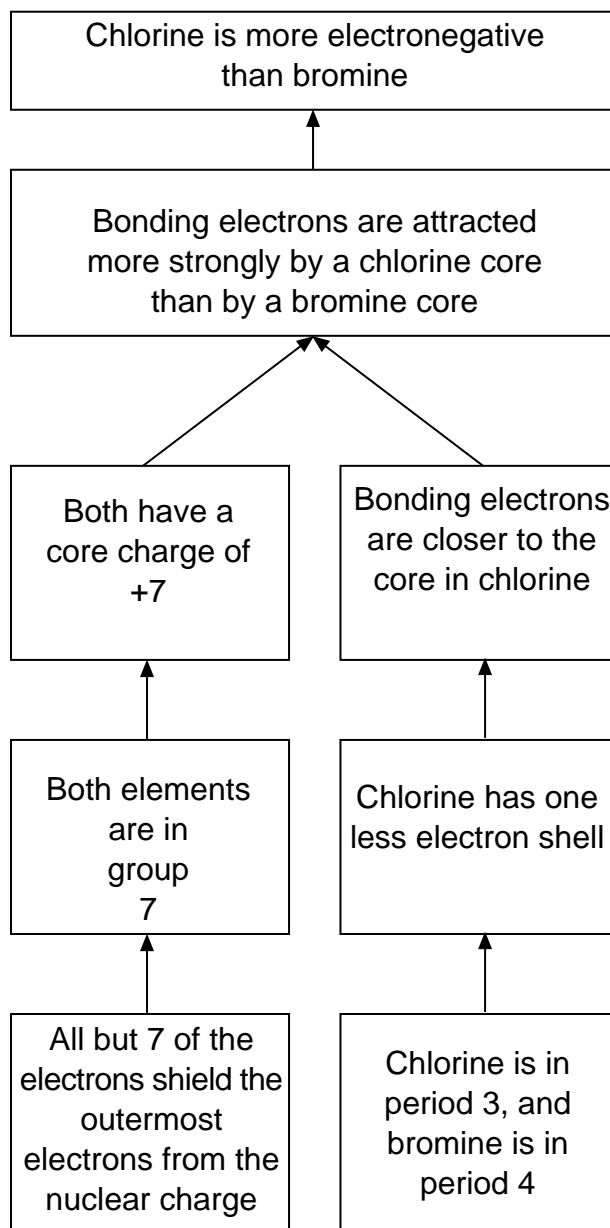
2. There is stronger bonding, called hydrogen bonding, between molecules of water (H_2O) than between molecules of hydrogen sulfide (H_2S).



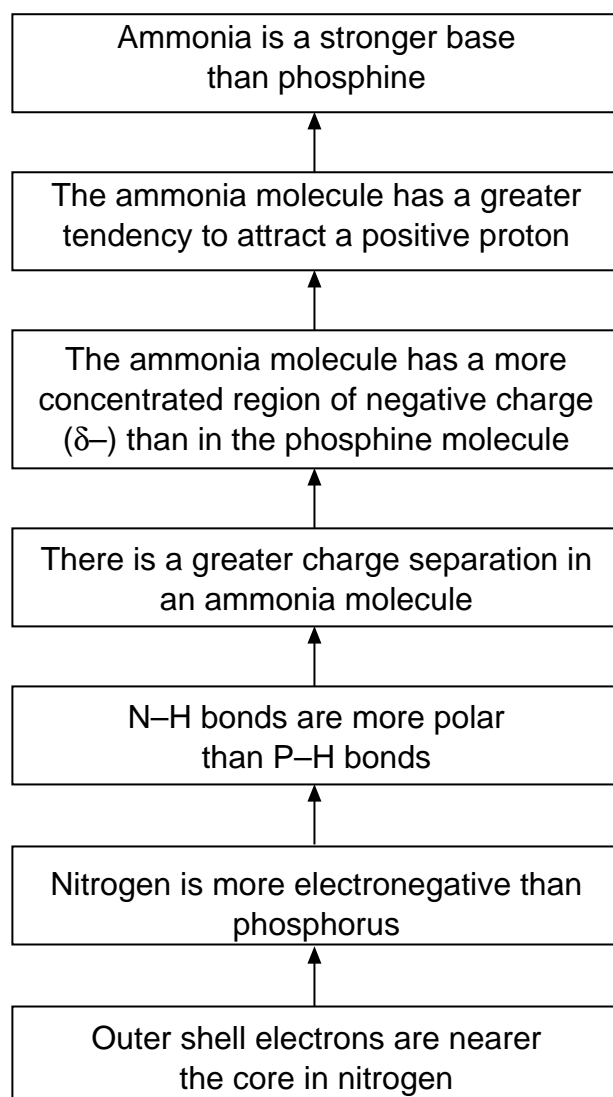
3. The nitrogen atom is smaller than the carbon atom (ie it has a smaller covalent radius - 0.074 nm compared to 0.077 nm).



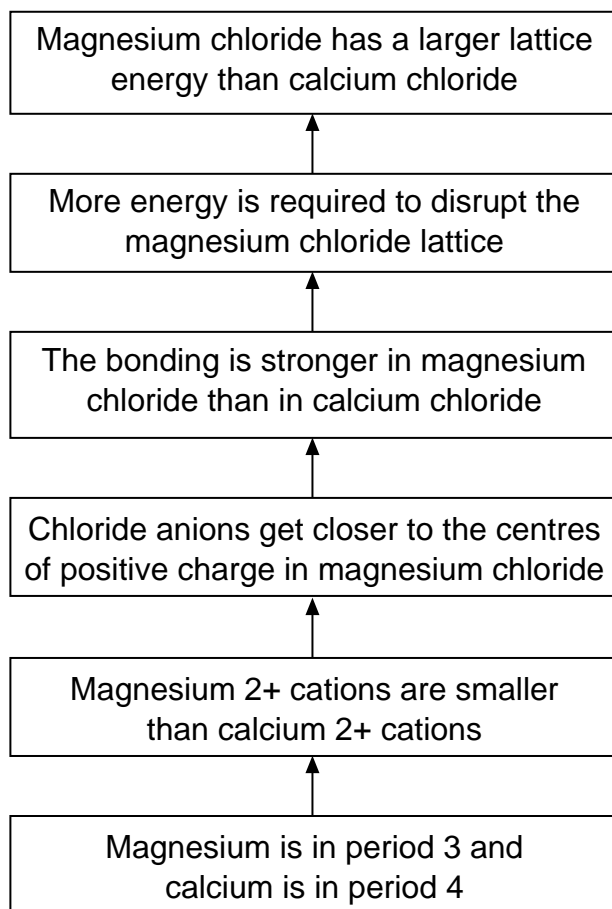
4. Chlorine is more electronegative than bromine.



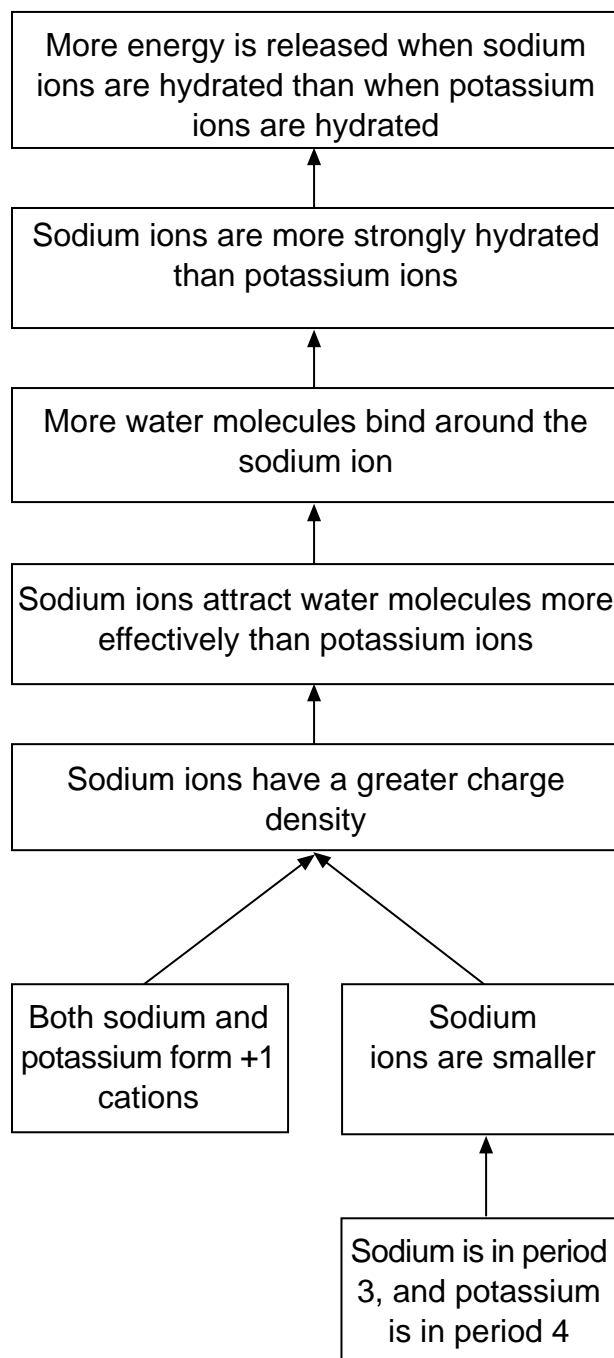
5. Ammonia (NH_3) is a stronger base than phosphine (PH_3).



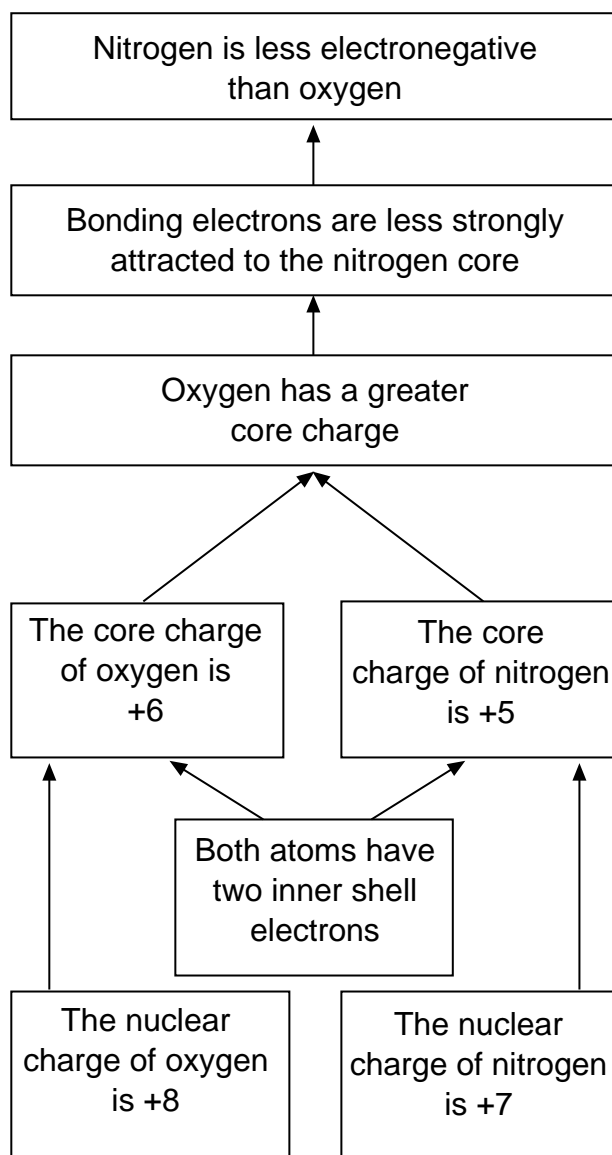
6. Magnesium chloride has a larger lattice energy (2489 kJ mol^{-1}) than calcium chloride (2197 kJ mol^{-1}).



7. More energy is released when sodium ions are hydrated (390 kJmol^{-1}) than when potassium ions are hydrated (305 kJmol^{-1}).



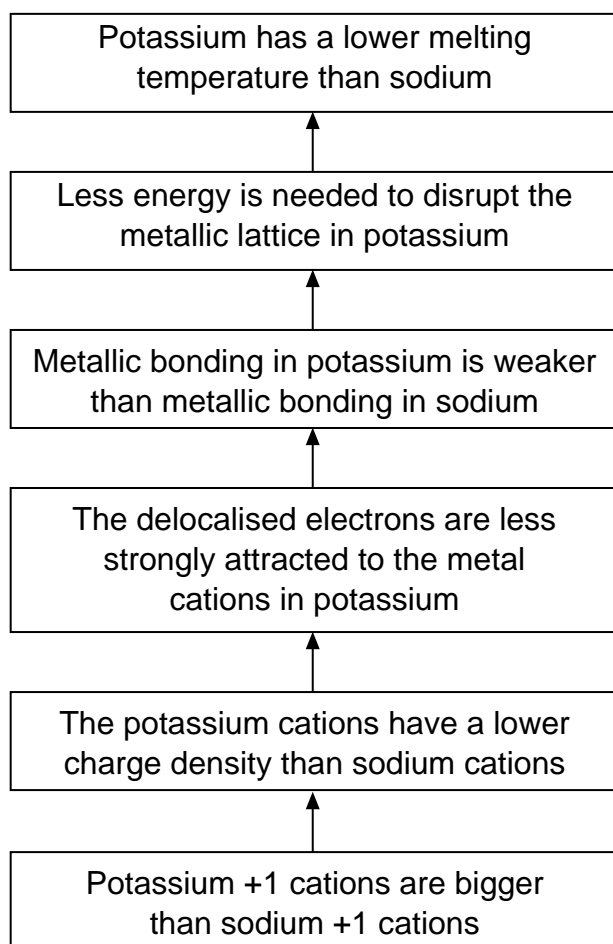
8. Nitrogen is less electronegative than oxygen.



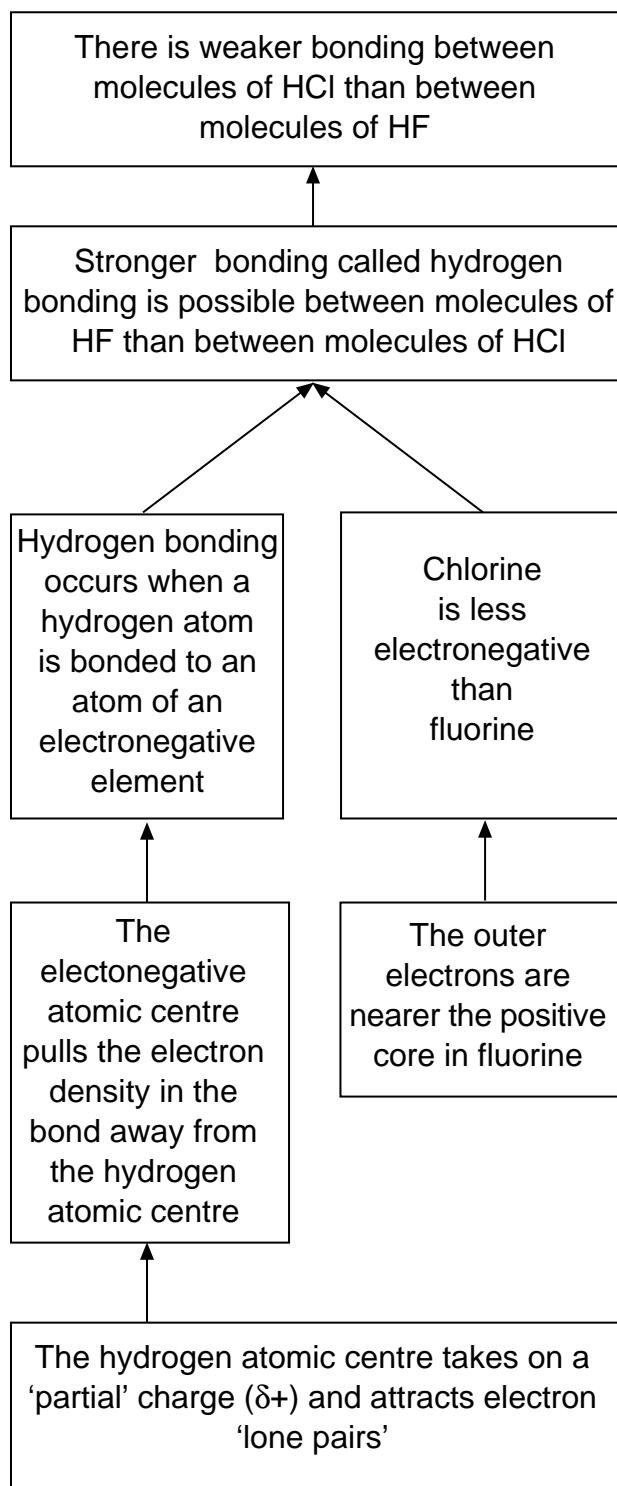
Examples of chemical explanations (2)

The following schemes may be useful as the basis for explaining the eight included in the worksheet **Explaining chemical phenomena (2)**

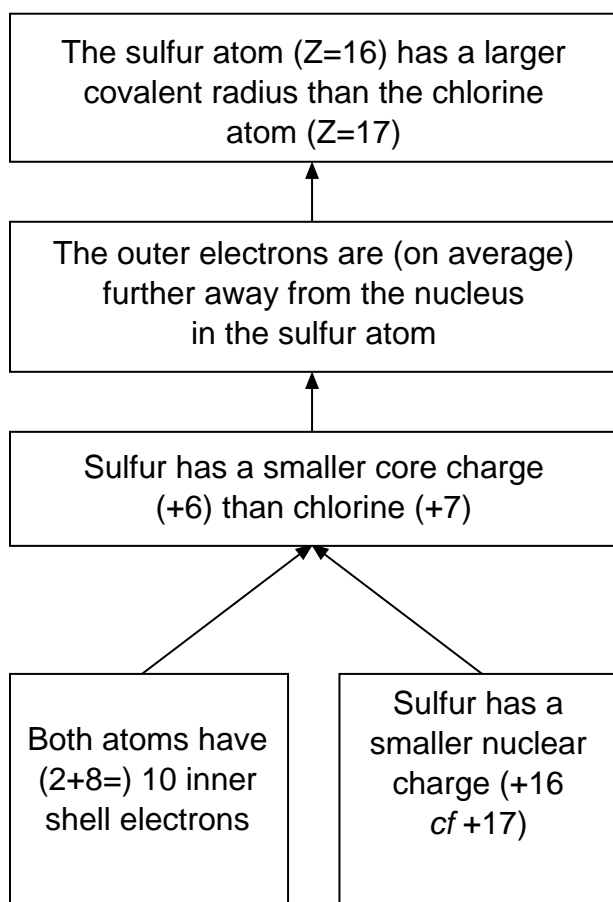
1. Potassium has a lower melting temperature (336 K) than sodium (371 K).



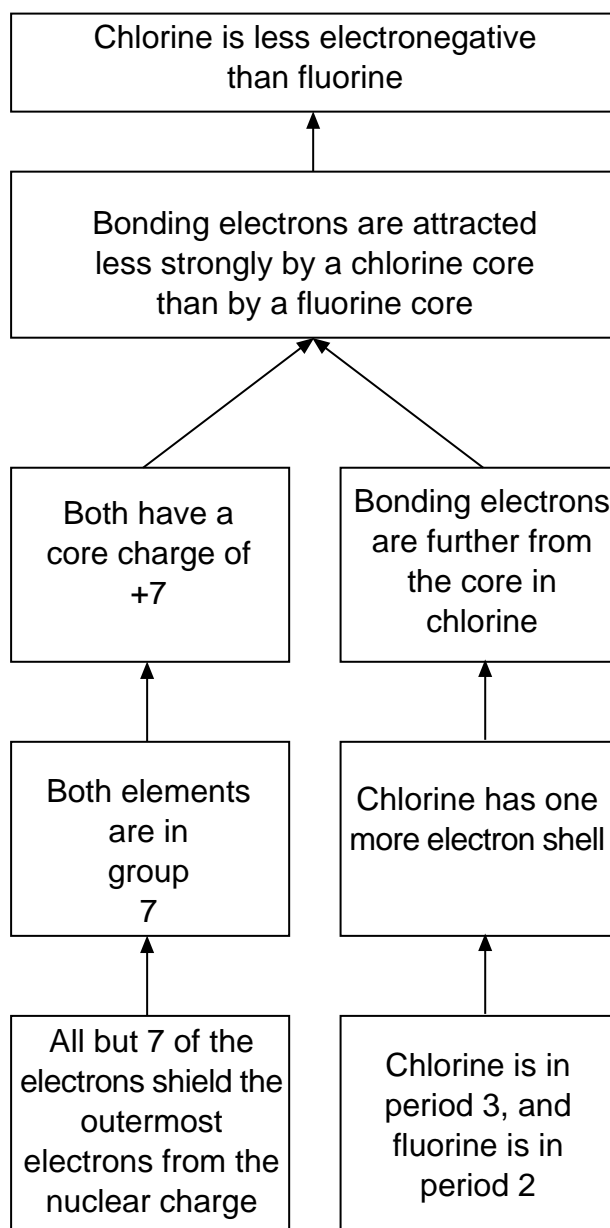
2. There is weaker bonding between molecules of hydrogen chloride (HCl) than between molecules of hydrogen fluoride (HF).



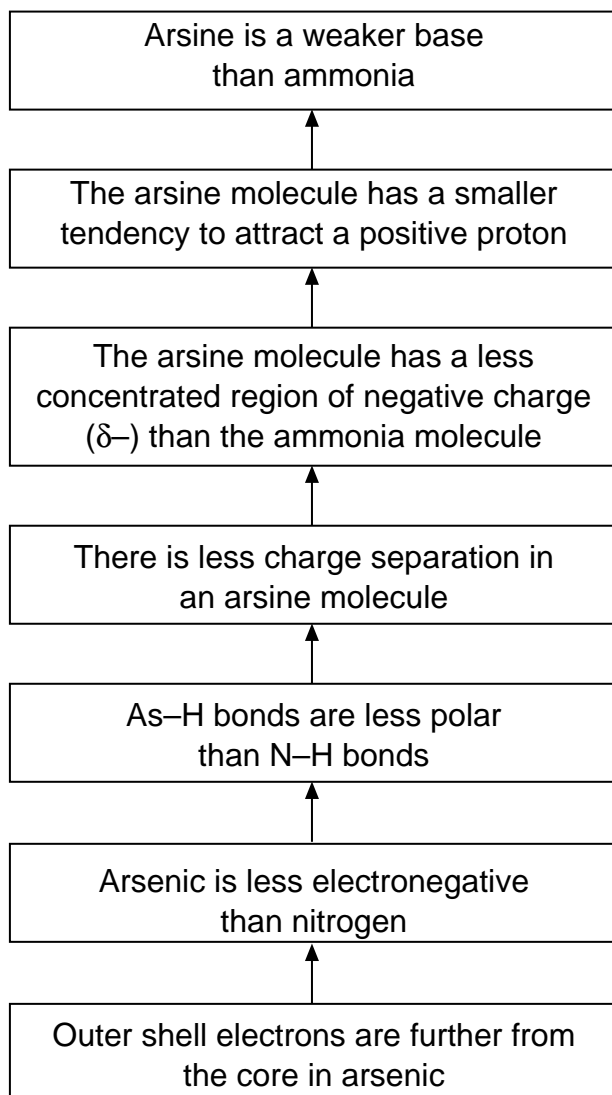
3. The sulfur atom is larger than the chlorine atom (ie it has a greater covalent radius – 0.104 nm compared to 0.099 nm).



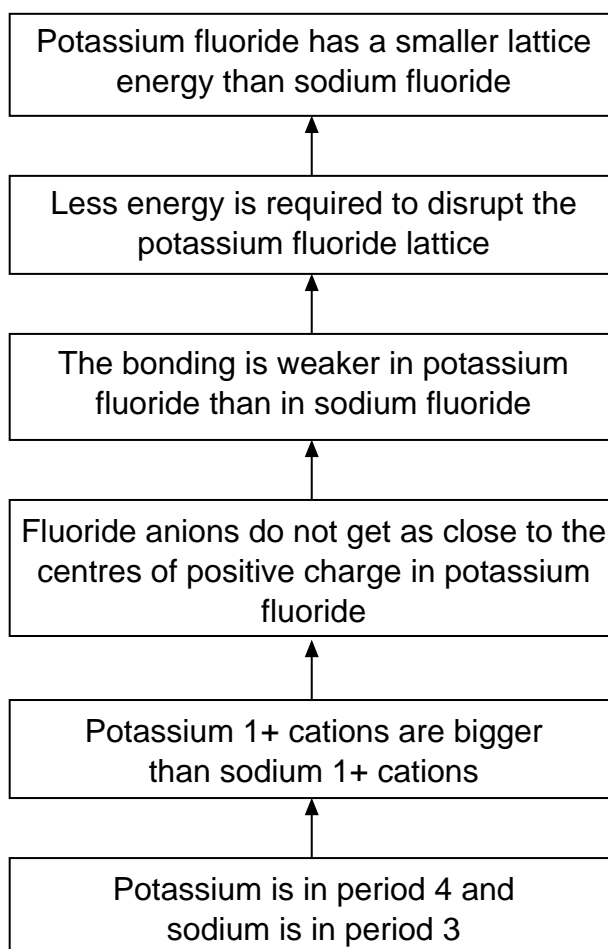
4. Chlorine is less electronegative than fluorine.



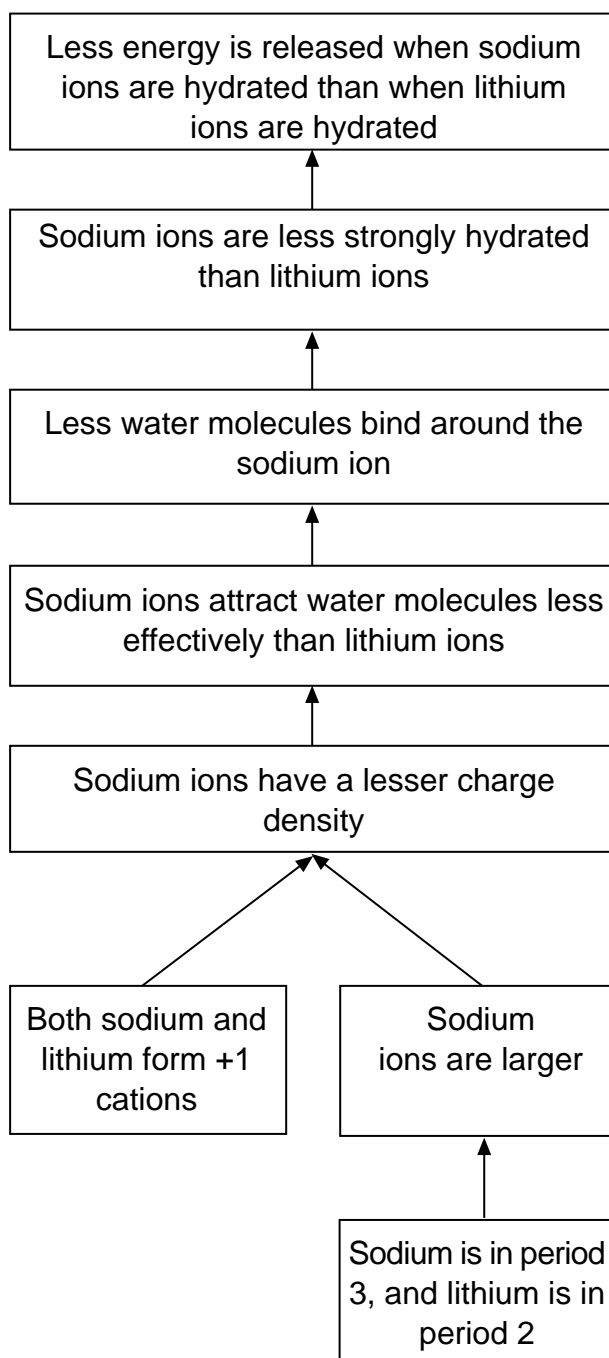
5. Arsine (AsH_3) is a weaker base than ammonia (NH_3).



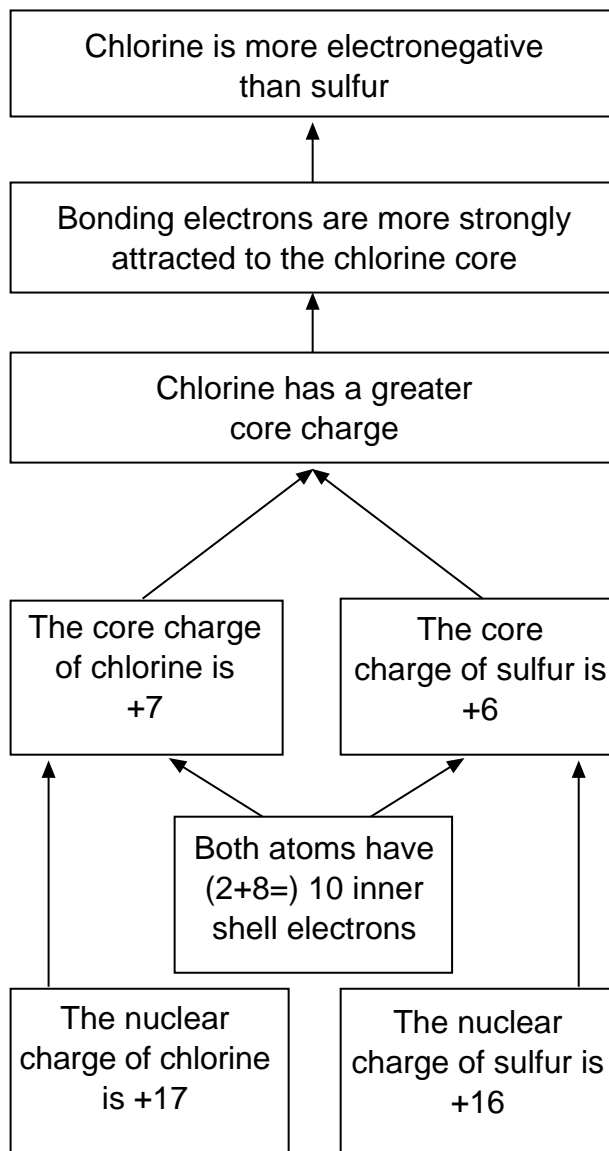
6. Potassium fluoride has a smaller lattice energy (813 kJmol^{-1}) than sodium fluoride (915 kJmol^{-1}).



7. Less energy is released when sodium ions are hydrated (390 kJmol^{-1}) than when lithium ions are hydrated (499 kJmol^{-1}).



8. Chlorine is more electronegative than sulfur.



Explaining chemical phenomena (1)

Chemists use their models and theories to try and explain phenomena about chemical systems. Suggest an explanation for each of the following (you may find it useful to refer to a periodic table):

1. Lithium has a higher melting temperature (454 K) than sodium (371 K).

2. There is stronger bonding, called hydrogen bonding, between molecules of water (H_2O) than between molecules of hydrogen sulfide (H_2S).

3. The nitrogen atom is smaller than the carbon atom (*ie* it has a smaller covalent radius – 0.074 nm compared to 0.077 nm).

4. Chlorine is more electronegative than bromine.

5. Ammonia (NH_3) is a stronger base than phosphine (PH_3).

6. Magnesium chloride has a larger lattice energy (2489 kJmol^{-1}) than calcium chloride (2197 kJmol^{-1}).

7. More energy is released when sodium ions are hydrated (390 kJmol^{-1}) than when potassium ions are hydrated (305 kJmol^{-1}).

8. Nitrogen is less electronegative than oxygen.

Constructing chemical explanations

Chemists use models and theories to try and explain phenomena about chemical systems. Although chemists seems to use a wide range of different models and theories, many of them are based on the same few basic principles.

If you can learn about these basic ideas you can use them as 'tools' to build up chemical explanations.

Some basic ideas used in explaining chemistry

The importance of size and charge

A large number of chemical phenomena can be explained, at least partly, in terms of simple ideas like the size and charge on ions or other particles.

Charge density

If two ions have the same charge, but are different in size, then the smaller one is said to have a greater density of charge. The ion with the greater density of charge can often have a greater effect – if it can get up close to other ions or molecules.

An ion with greater charge density can form a stronger bond with an oppositely charged ion. This can lead to a more stable ionic lattice, which therefore requires more energy to disrupt. (So the lattice energy of magnesium chloride is greater than the lattice energy of calcium chloride - as the Mg^{2+} ion, which is smaller, has a greater charge density than the Ca^{2+} ion, even though they have the same charge.)

If the ions are of similar size, but have a different charge the one with the greater charge will have the larger charge density, and may be able to form stronger bonds.

When ionic materials dissolve in water the ions are hydrated (surrounded by water molecules which bond to them). The greater the charge density of an ion the more water molecules will bond to it, and the more energy will be released when a material with that type of ion dissolves.

These ideas do not always help us predict what will happen in experiments, as sometimes there are several effects operating at once. For example, an ion with a greater charge density can be hydrated more (which would make the material more soluble) but will usually bond more strongly to oppositely charged ions (which would make the material harder to dissolve!)

In some books the terms charge:size (charge to size ratio) or charge:volume (charge to volume ratio) may be used instead of charge density.

Core charge

Many chemical processes can be – at least partly – explained in terms of the charges in the ions or molecules involved. Atoms are neutral, but separate atoms are seldom involved in chemical processes. Usually we are concerned with ions or molecules.

In what ways are ions and molecules like atoms, and how are they different?

Atoms may be thought of as a positive nucleus surrounded by several shells of electrons. (Of course, the electronic structure is more complicated than that, with different types of orbitals. However, it is often useful to think in terms of shells.) Most of the time the nuclei of the atoms do not change (and when they do this is studied by physicists). Usually only the outermost shell of electrons, the valence shell, is changed in chemical processes. The nucleus and all the inner shells are usually not significantly changed.

The term core is used to describe the nucleus of an atom, plus all the electrons that are not in the outer (valence) shell.

The charge on an atomic core is called the core charge.

It is often useful to know what the core charge is. The core charge will equal the positive charge on the nucleus plus the negative charge of all the inner-shell electrons.



The table shows how to calculate core charge.

Complete the table.

Element E	Atomic Number Z	Number of protons n_p	Number of electrons n_e	Electronic configuration e.c.	Number of outershell electrons n_{ve}	Number of core electrons $n_{ce} (=n_e - n_{ve})$	To calculate core charge $n_p - n_{ce} =$	Core charge c.c.
H	1	1	1	1	1	0	$1-0 =$	+1
He	2	2	2	2	2	0	$2-0 =$	+2
Li	3	3	3	2.1	1	2	$3-2 =$	+1
Be	4	4	4	2.2	2	2	$4-2 =$	+2
B	5	5	5	2.3	3	2	$5-2 =$	+3
C	6	6	6	2.4		2		+4
N	7	7	7		5	2	$7-2 =$	+5
O	8	8	8	2.6	6	2	$8-2 =$	
F	9	9	9	2.7				+7
Ne	10	10	10	2.8			$10-2 =$	
Na	11	11	11	2.8.1	1	10	$11-10 =$	+1
Mg				2.8.2	2	10	$12-10 =$	+2
Al	13	13	13	2.8.3		10		+3
Si	14			2.8.4	4			+4
P				2.8.5		10		
S					6	10		
Cl				2.8.7				+7
Ar	18	18	18	2.8.8	8	10	$18-10 =$	+8
K	19			2.8.8.1	1	18	$19-18 =$	
Ca	20	20	20		2			+2

The diagram below shows the symbols for the first 20 elements. Using the table on the previous page, complete the diagram by adding the core charges that are not shown.

Can you spot any pattern?

Core charge for the first 20 elements							
H +1							He +2
Li +1	Be +2	B	C +4	N +5	O	F +7	Ne +8
Na +1	Mg +2	Al +3	Si +4	P	S	Cl +7	Ar +8
K	Ca +2						

Electronegativity

One of the most useful chemical concepts is that of electronegativity.

Electronegativity is the tendency of an element to attract the bonding electrons towards itself in compounds.

The electronegativity of an element depends upon how strongly the outer (valence) shell electrons are attracted to the core. The greater the charge on the core, and the nearer the outer shell of electrons are, the more strongly they are bound to the core.

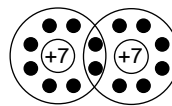
Electronegativity is therefore greater at the top of a group (where the outer shell of negatively charged electrons is pulled closest to the positively charged nucleus) and to the right of a period (where the core charge is greatest):

Approximate core charge density for some of the elements							
H ⊕ ⁺¹							
Li ⊕ ⁺¹	Be ⊕ ⁺²	B ⊕ ⁺³	C ⊕ ⁺⁴	N ⊕ ⁺⁵	O ⊕ ⁺⁶	F ⊕ ⁺⁷	
Na ⊕ ⁺¹	Mg ⊕ ⁺²	Al ⊕ ⁺³	Si ⊕ ⁺⁴	P ⊕ ⁺⁵	S ⊕ ⁺⁶	Cl ⊕ ⁺⁷	
K ⊕ ⁺¹	Ca ⊕ ⁺²						

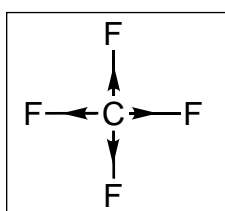
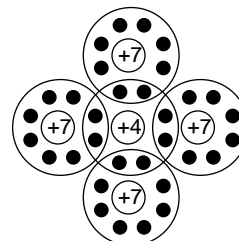
Bond polarity in terms of electronegativity

Where the electrons in a bond are pulled equally by both cores, the bond is non-polar.

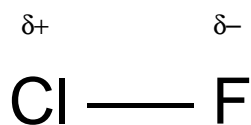
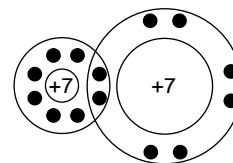
For example in F_2 both the atoms of fluorine have cores of the same size and charge.



However, in the molecule of CF_4 the fluorine atoms have a more highly charged core, and the bonding electrons are pulled closer to the fluorine cores than carbon core. The bonds are polar. This can be represented as:



The inter-halogen compound ClF also has a polar bond. Although the cores of both atoms have the same charge, the fluorine core has a higher charge density. This can be represented as:



Building up chemistry explanations

Many of the explanations we construct in chemistry use ideas such as charge density, core charge and electronegativity. Many explanations can be built up using just a few basis ideas. Certain key phrases can be used as tools for building up explanations. (This does not mean you can just pick any key phrase: you have to understand the chemistry, and select the right phrases for a particular explanation!)

Consider the question: why do water molecules bond together?

Water molecules bond together because they are polar.

Water molecules are polar because the hydrogen-oxygen bond is polar.

The hydrogen-oxygen bond is polar because oxygen is more electronegative than hydrogen.

Oxygen is more electronegative than hydrogen because oxygen has a larger core charge.

This is not a 'complete' explanation. It would be possible to explain in more detail about the core charge (eg oxygen has a core charge of +6 because it has a nucleus of charge +8, partly shielded by 2 electrons in the core). It is also important to know that a molecule with polar bonds is not always a polar molecule! (So the molecule of CF_4 discussed above has four polar bonds, but overall the molecule is non-polar.) The explanation above could be improved by adding:

... Water molecules are polar because the hydrogen-oxygen bond is polar, and the water molecule has two polar bonds which do not cancel out ...

This theme could also be continued...

... The two polar bonds do not cancel because the water molecule is angular.

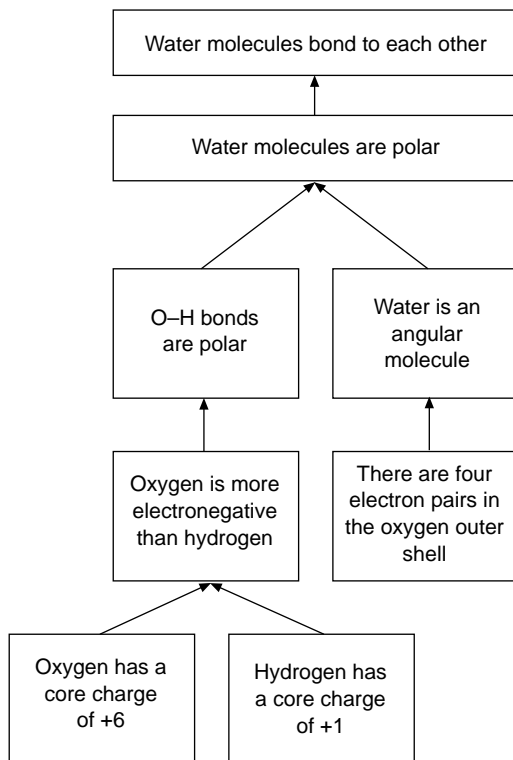
The water molecule is angular because there are four electron pairs in the oxygen outer shell.

There are two non-bonding (lone) pairs as well as the two pairs of bonding electrons ...

So even a simple question could have a very complicated answer if we want to give a full and detailed explanation. You do not normally need to do this, although it can be good practice in testing how well you understand your chemistry.

Charting your explanations

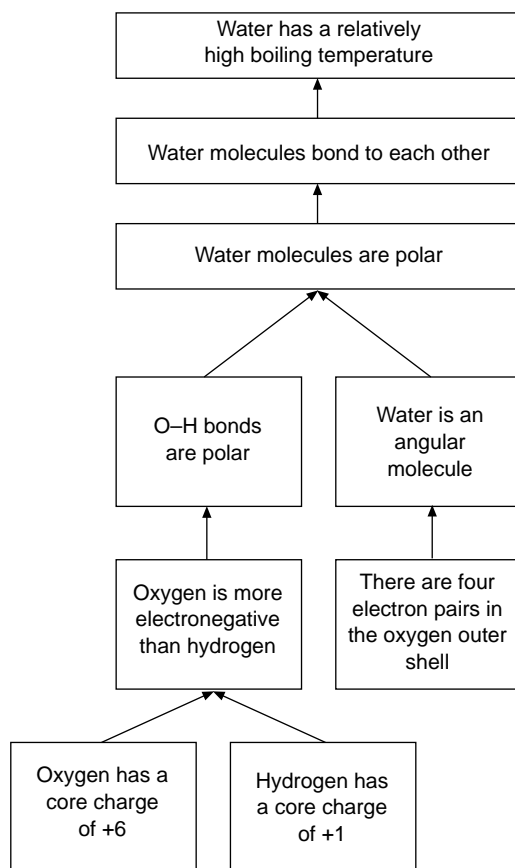
If some explanations seem rather complicated, you may find it helps to break the explanation down into steps, which can be put into a flow chart. In the example below, the phenomenon to be explained is written at the top of the box, and each arrow may be read as a 'because'.



Although such a scheme may seem complicated, it helps to learn to think about the individual steps in the explanations. If you can understand the steps you can learn to put together such schemes.

For example consider the question: why does water have a higher boiling temperature than would be predicted from its molecular mass?

You may know that it is because the hydrogen bonding in water holds the molecules together, so that more energy is needed to separate the molecules. In other words, we can amend the scheme above.



Some key phrases

The following phrases are examples of some of those that may be useful in constructing explanations (you may want to add to this list):

- has strong(er)/weak(er) bonding
- is more/less electronegative
- has a higher/lower charge density
- has a larger/smaller core charge
- electrons are nearer/further from the nucleus

Explaining chemical phenomena (2)

Chemists use their models and theories to try and explain phenomena about chemical systems. Suggest an explanation for each of the following (you may find it useful to refer to a Periodic Table).

1. Potassium has a lower melting temperature (336 K) than sodium (371 K).

2. There is weaker bonding between molecules of hydrogen chloride (HCl) than between molecules of hydrogen fluoride (HF).

3. The sulfur atom is larger than the chlorine atom (*ie* it has a greater covalent radius – 0.104 pm compared to 0.099 pm).

4. Chlorine is less electronegative than fluorine.

5. Arsine (AsH_3) is a weaker base than ammonia (NH_3).

6. Potassium fluoride has a smaller lattice energy (813 kJmol^{-1}) than sodium fluoride (915 kJmol^{-1}).

7. Less energy is released when sodium ions are hydrated (390 kJmol^{-1}) than when lithium ions are hydrated (499 kJmol^{-1}).

8. Chlorine is more electronegative than sulfur.

