Physical chemistry 1

Atomic structure

- The energy it takes to remove electron can be measured and is called the ionisation energy because as electrons are removed, atoms become positive ions.
- Ionisation energy (IE) is the energy required to remove 1 mole of electrons from 1 mole of atoms in the gaseous state and is measured in $kJmol^{-1}$.
- It is written as $X(g) \rightarrow X^{+}(g) + e^{-}$ (1^{st} IE)

<u>Removing electrons 1 by 1</u>

- You can measure the energies required to remove electrons 1 by 1 starting from the outer shell and working inwards.
- The 1^{st} electron needs the least amount of energy because it's being removed from a neutral atom. This is the 1^{st} IE.
- The 2^{nd} electron needs more energy than the 1^{st} because it's being removed from a +1 ion, meaning it's attracted more strongly. This is the 2^{nd} IE.
- The 3^{rd} needs even more and so on.
- This is called successive ionisation energies.
- 1^{st} IE = $X(g) \rightarrow X^{+}(g) + e^{-}$
- 2^{nd} IE = $X^{+}(g) \rightarrow X^{2+}(g) + e^{-}$
- 3^{rd} IE = $X^{2+}(g) \rightarrow X^{3+}(g) + e^{-}$
- E.g. Sodium

Electron removed	1	2	3	4	5	6	7	8	9	10	11
Ionisation energy ($kJmol^{-1}$)	496	4,563	6,913	9,544	13,352	16,611	20,115	25,491	28,934	141,367	159,079

- Notice that the 2^{nd} IE isn't $Na(g) \rightarrow Na^{2+}(g) + 2e^{-}$. This would be the 1^{st} and 2^{nd} IE together.
- 1 electron is relatively easy to remove then comes a group of 8 that are more difficult to remove and then 2 which are very difficult to remove.
- This suggests that Na has:
    - 1 electron far away from the positive nucleus (easy to remove).
    - 8 electrons nearer to the positive nucleus (harder to remove).
    - 2 electrons very close to the positive nucleus (difficult to remove).
- A graph of this tells you about the number of electrons in each main level and, with a good scale, the sublevels too.
- You can find the number of electrons in each energy level for any element by looking at the successive energy levels (specifically at the jumps).

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Trends in the IE across a period

- Also gives information about number of electrons in the main shells and the sublevels.
- IEs generally increase across a period because the nucleic charge increases.
- The element that has an electron in a new orbital will have slightly less IE despite the increase in nucleic charge (e.g. Magnesium to Aluminium) because the new orbital has slightly higher energy, needing less energy to remove the electron.
- The element which has enough electrons that 1 orbital has 2 electrons will have slightly less IE despite the increase in nucleic charge because the electrons repel, making it easier to lose 1 of them.
- These are evidence of sublevels, predicted by quantum theory and the Schrodinger's equation.

Trends in IE down a group

- There is a general decrease in IEs down a group because the outer electron gets further away from the nucleus.
- The increase in nucleic charge doesn't make it harder to remove the electron because electron shielding causes the positive charge 'felt' by the electron to be less than the nuclear charge.

Electron shielding

- The electrons in between the outer shell and the nucleus effectively act as a part of the nucleus, cancelling some of the positive charge.