WebMO is an interactive web programme which can be used alongside your A-Level studies in areas such as shapes of molecules, the understanding of electronegativity in covalent bonds and IR and NMR spectroscopy.

After login, the first screen you will encounter is the WebMO Job Manager which displays all the jobs which have been recently processed worldwide. You can view different jobs by clicking the formula or the magnifying glass.

Next, you can begin to build your molecule on the “Build Molecule” screen. Click “Build” then select “Other”. A periodic table will appear and you can choose your element. Alternatively, press the letter of the element on the keyboard. Click on the screen to place each atom. You can link atoms by dragging the mouse from one atom to another. To optimise the geometry of the molecule, click the “Clean Up” drop down menu and select the “Geometry” option.

Simply press the right hand arrow and choose a computational engine to run the calculation on your molecule.

Now add your name or initials to the end of the formula so you can identify it on the Job Manager page and select “Geometry Optimisation” in the drop down box beneath it.

Finally, click the right hand arrow again to run the calculation on your molecule.