=Marking=

Note: All grades and comments are provisional and subject to change until your grades are officially returned via blackboard. Please do not contact anyone about anything to do with the marking of this lab until you have received your grade from blackboard.

==Wiki structure and presentation 1/1 ==

Is your wiki page clear and easy to follow, with consistent formatting?

YES

Do you effectively use tables, figures and subheadings to communicate your work?

YES

==NH3 1/1 ==

Have you completed the calculation and given a link to the file?

YES

Have you included summary and item tables in your wiki?

YES

Have you included a 3d jmol file or an image of the finished structure?

YES

Have you included the bond lengths and angles asked for?

YES

Have you included the “display vibrations” table?

YES

Have you added a table to your wiki listing the wavenumber and intensity of each vibration?

YES

Did you do the optional extra of adding images of the vibrations?

YES

Have you included answers to the questions about vibrations and charges in the lab script?

YES

== N2 and H2 0.5/0.5 ==

Have you completed the calculations and included all relevant information? (summary, item table, structural information, jmol image, vibrations and charges)

YES

==Crystal structure comparison 0.5/0.5 ==

Have you included a link to a structure from the CCDC that includes a coordinated N2 or H2 molecule?

YES

Have you compared your optimised bond distance to the crystal structure bond distance?

YES

==Haber-Bosch reaction energy calculation 1/1==

Have you correctly calculated the energies asked for? $\Delta E=2*E(NH3)-[E(N2)+3*E(H2)]$

YES

Have you reported your answers to the correct number of decimal places?

YES

Do your energies have the correct +/- sign?

YES

Have you answered the question, Identify which is more stable the gaseous reactants or the ammonia product?

YES

== Your choice of small molecule 5/5 ==

Have you completed the calculation and included all relevant information?

YES

Have you added information about MOs and charges on atoms?

YES

== Independence 1/1 ==

If you have finished everything else and have spare time in the lab you could:

Check one of your results against the literature, or

Do an extra calculation on another small molecule, or

Do some deeper analysis on your results so far

Common comments

However you have given a bond angle of 180 for N2 and H2, there are no bond angles in diatomic molecules. Bond angles involve exactly 3 atoms.

most answers are correct. However there are only 2 visible peaks in the spectra of NH3, due to the low intensity of the other 2 peaks. (See infrared column in vibrations table.)

However you got the bond lengths and angles wrong because you measured them on the input structure not the optimised structure in the final step.

You have left all the jmol captions as the default “test molecule” this gives the reader no information.

YES, you have included too many d.p. though, for this method you should report angles to the nearest degree and bond lengths in A to 2 d.p.

[[File:rr1210-sih4-mos.png|400px|thumb|SiH4 MOs]]

[https://wiki.ch.ic.ac.uk/wiki/index.php?title=Mod:CO2_MO_explanation See this wiki page for more details on the CO2 MOs.]