Computational Chemistry Labs 2011-12

http://wiki.ch.ic.ac.uk/wiki/index.php?title=Main_Page

Find minima to calculate what you can't see .: beneficial to do first

IR spectra from molybdenum last year

Water in sample

1 – organic = molecular mechanics

2- inorganic - qm

3 – transition states

Late breaking news

Demonstrator: 12-1 and 2-4 in tutorial room (staff: 2-3)

2 – tricia hunt

3- bearpark

Deadlines

http://wiki.ch.ic.ac.uk/wiki/index.php?title=Mod:mechanics

mm: molecular mechanics – chembio 3d

http://wiki.ch.ic.ac.uk/wiki/index.php?title=Mod:organic

Monosaccharide chemistry: glycosidation

Expected to have these moveable molecules in our wiki pages

SCAN: if molecules too big

Mod 2 – some calc overheat computer

Module 1

Calculations second to minutes

Module 2

Need to use SCAN

If it doesn't work after 3-4 times ASK

4-6 hours for these .: overnight

Schrodinger equation

- Hamiltonian: e-e exchange and coulomb part
    - Coulombic = permitivity, charges, distance
- Nuclear nuclear repulsion
- E-n attraction
- Kinetic energy (electrons)

H = Vee + Vnn + Vne + Ek

For wavefunction use hydrogenic atomic orbitals – in atkins

Coefficient, exponent and polynomial

➔ Describe orbitals

Use gaussian functions and the more the better/more accurate = because easy to work with

Usually one HAO = 3 functions

2 things to vary = how heavily weighted and how wide

Force field – proteins

Dft lda hf – can use qm

Dft – density

Correlation – important once start to break bonds

Qm fully – have nuclei with wavefunction as well

➔ Don't use last 2

Will use chem3d and gaussian

Different systems available because of the type of approximations we use

Gaussian – orcha is optional and free

Ave bond – 100-300 kj mol-1

Auccuracy and error reporting

Accuracy decimal places crystal structure

2 for hydrogen

3-4 for others

Angles 2-3 degrees

Hartrees and atomic units → kJ mol-1

Ammonia – NH3

# degrees of freedom

4 atoms each with x,y,x = 12 different numbers to put 4 atoms somewhere

3 coord redundant (can turn and move without changing)

= 6

Increase #atoms = increase#degrees of freedom

Hf: fairly accurate energy surfaces but not necessarily a good energy difference

Sto-3g: slater type obitals

Opt freq – code

Use derivatives to get to the bottom of a hill

http://www.huntresearchgroup.org.uk/teaching.html

1: singlet

Relationship force gradient : equivalent (mass term too)

No qm definition of a bond .: ignore bonds b/c draws bonds based on distance

http://wiki.ch.ic.ac.uk/wiki/images/f/f3/Yr3lab_pes_rev.pdf