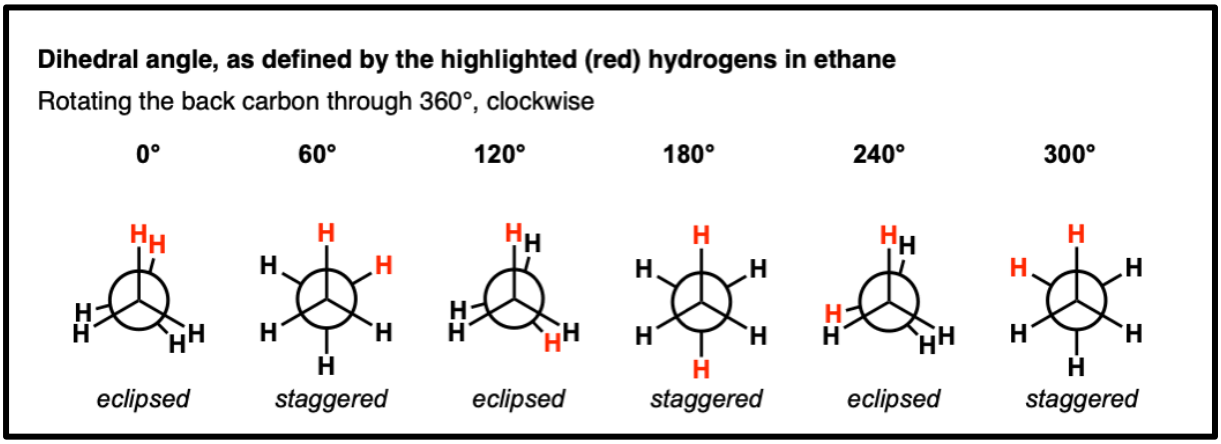
PC Lab: Kjem220: QM

Dihedral Scan

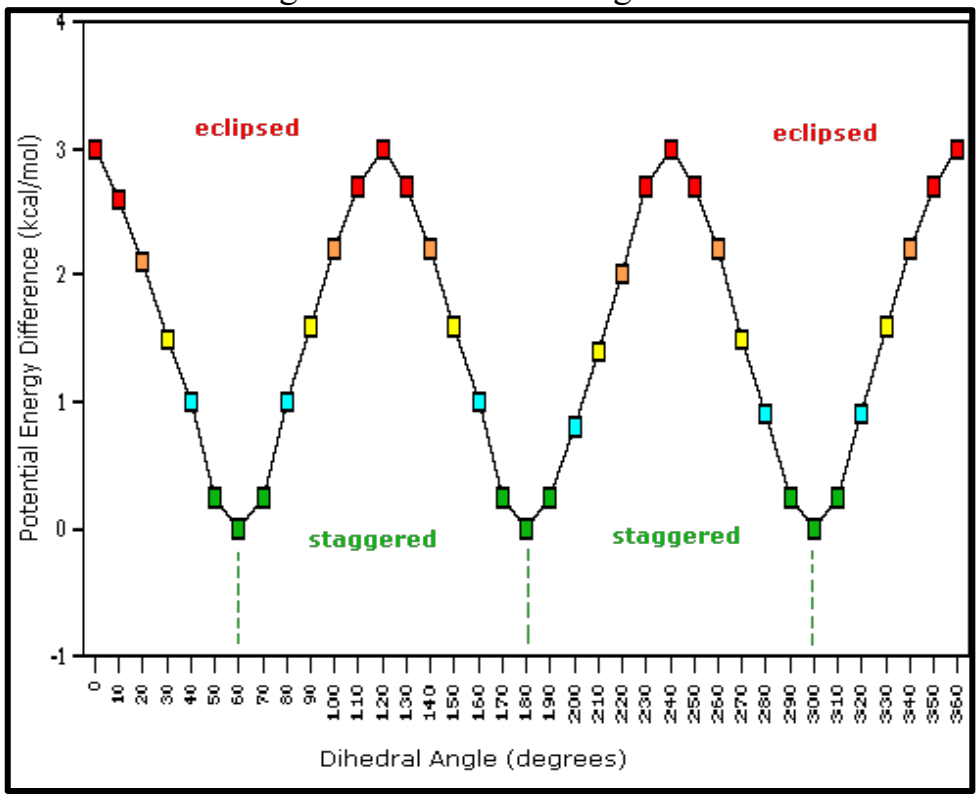
Ethane molecule: rotations around the C-C single bond in ethane molecule can lead to different conformations of the molecule. This is called conformational isomerism.

- Conformational isomers are same molecules that differ in rotation of one or more sigma bond.

- Different conformations of ethane:



- Plot of relative energies vs the dihedral angle around C-C bond:



Tasks:

- Perform a dihedral scan around the H-C-C-H dihedral for ethane molecule from 0 to 360 degrees in 42 steps using ORCA.
- Convert the energies to kcal/mol.
- Plot the relative energy of conformations with respect to the dihedral angle.
- Visualize the trajectory using Avogadro.
- Which conformation of ethane molecule is the most stable from your calculation?

  They are the staggered conformations at angles 61.3, 176 and 300

Potential energy surface (PES)

A potential energy surface describes the potential energy of the system based on different parameters (such as bond length, bond angle etc.) of the molecule. The surface defines the energy as a function of one or more parameters. If there is only one parameter used then, the PES is called a potential energy curve or simply energy profile.

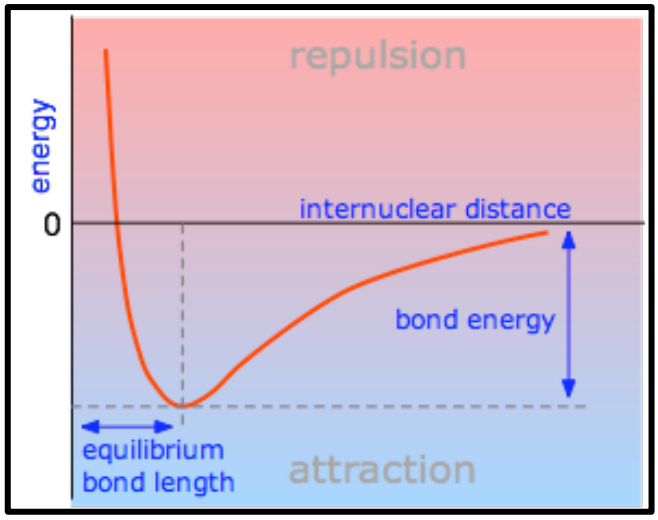
$$Total\ number\ of\ paramters\ on\ which\ PES\ depends:$$

$$For\ linear\ molecules = \ 3N - 5 \ \ (parameters)$$
$$For\ non - linear\ molecules = 3N - 6 \ \ (paramters)$$

$$where, N = number\ of\ atoms$$

1-D Potential Energy Surfaces

- For diatomic molecules, the energy of the system depends on the distance between them.
- The internuclear distance at which the potential energy is at its minimum corresponds to the bond length of the molecule.



Tasks:

- Plot the potential energy curve for H_2, HCl and H_2O using the bond distance as a function of potential energy (for water take one of the two O-H bonds).

- How many parameters are available to define the PES in case of water?

- Insert the values of equilibrium bond lengths in the table below:

Molecule	Equilibrium bond length (Å)
H_2	0.70
HCl	1.28
H_2O	0.90

References

https://chem.libretexts.org/Bookshelves/Organic_Chemistry/Organic_Chemistry_(McMurry)/03%3A_Organic_Compounds-_Alkanes_and_Their_Stereochemistry/3.06%3A_Conformations_of_Ethane

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