VIVEKANANDA COLLEGE

THAKURPUKUR

KOLKATA-700063

NAAC ACCREDITED ‘A’ GRADE

Topic: Stereochemistry: Conformational Analysis-1

Course Title: Organic Chemistry -2

Paper: CEMA-CC-2-3-TH

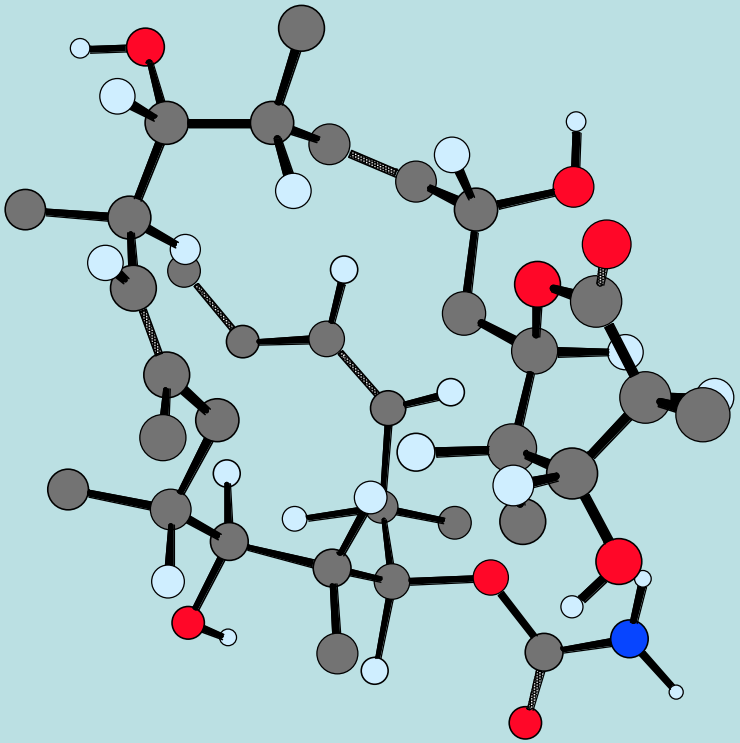
Unit: L-1

Semester: 2 (Hons)

Name of the Teacher: Yasin Nuree

Name of the Department: Chemistry

Conformational Analysis



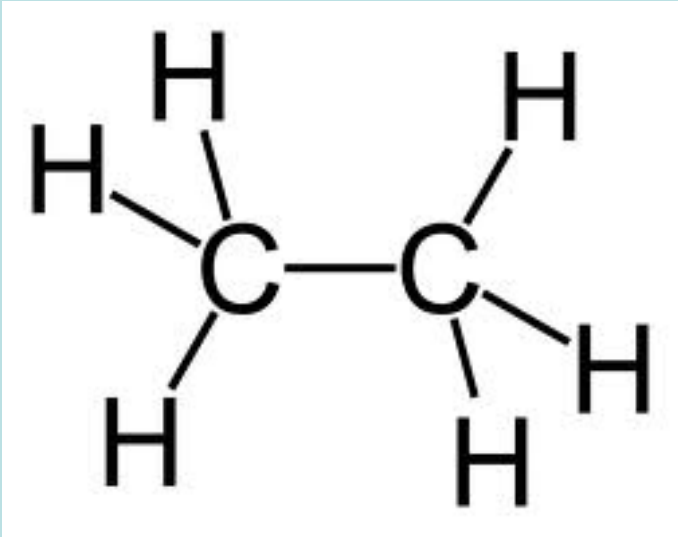
Carey & Sundberg: **Part A**; Chapter 3

Conformations of Alkanes and Cycloalkanes

- **Conformations** or **Conformers** or **Rotamers**;

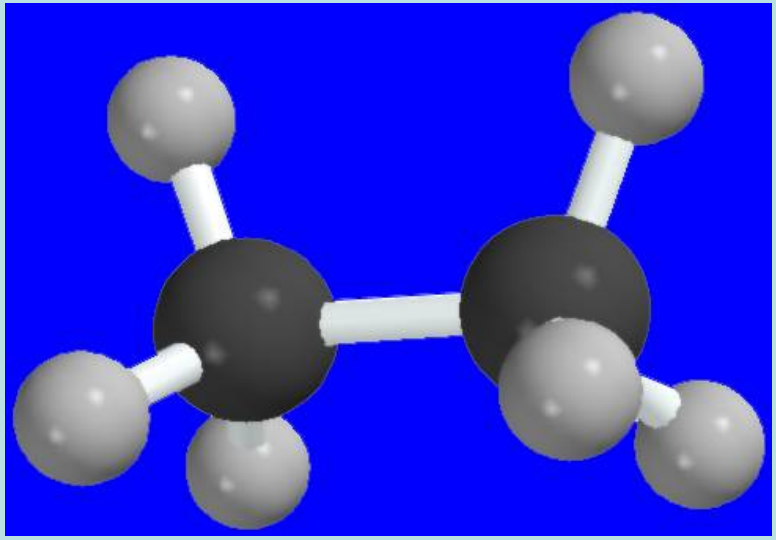
- Different spatial arrangements of a molecule that are generated by **rotation about single bonds**.

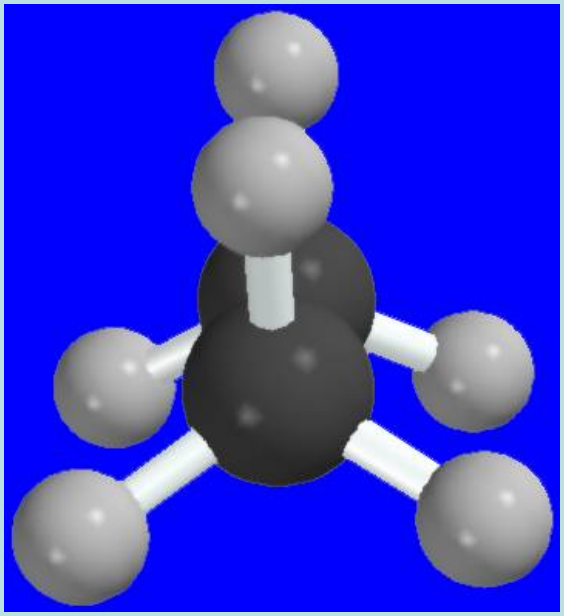
Ethane



Projection Formulas ?

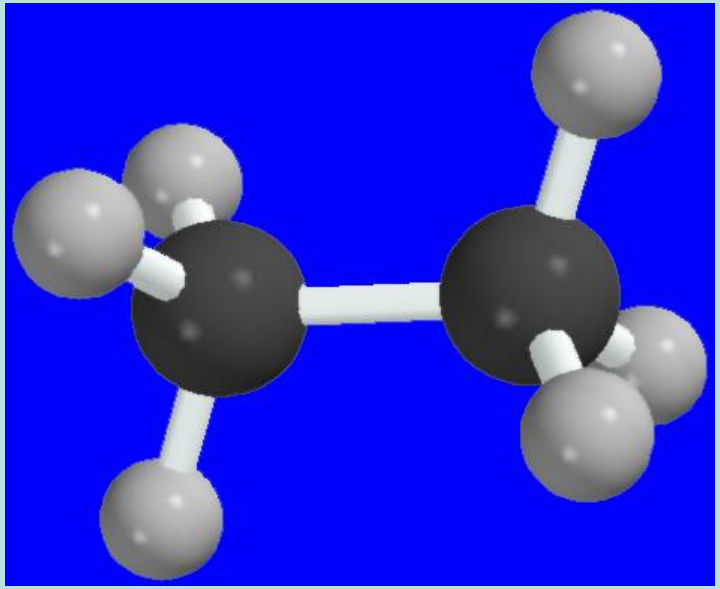
Ethane

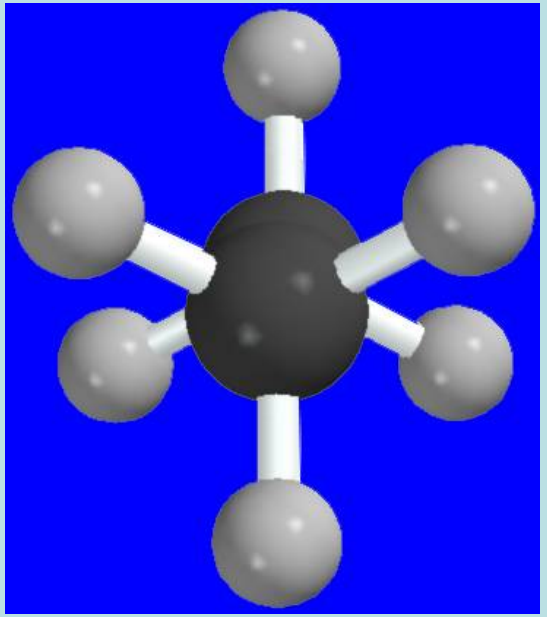




- eclipsed conformation

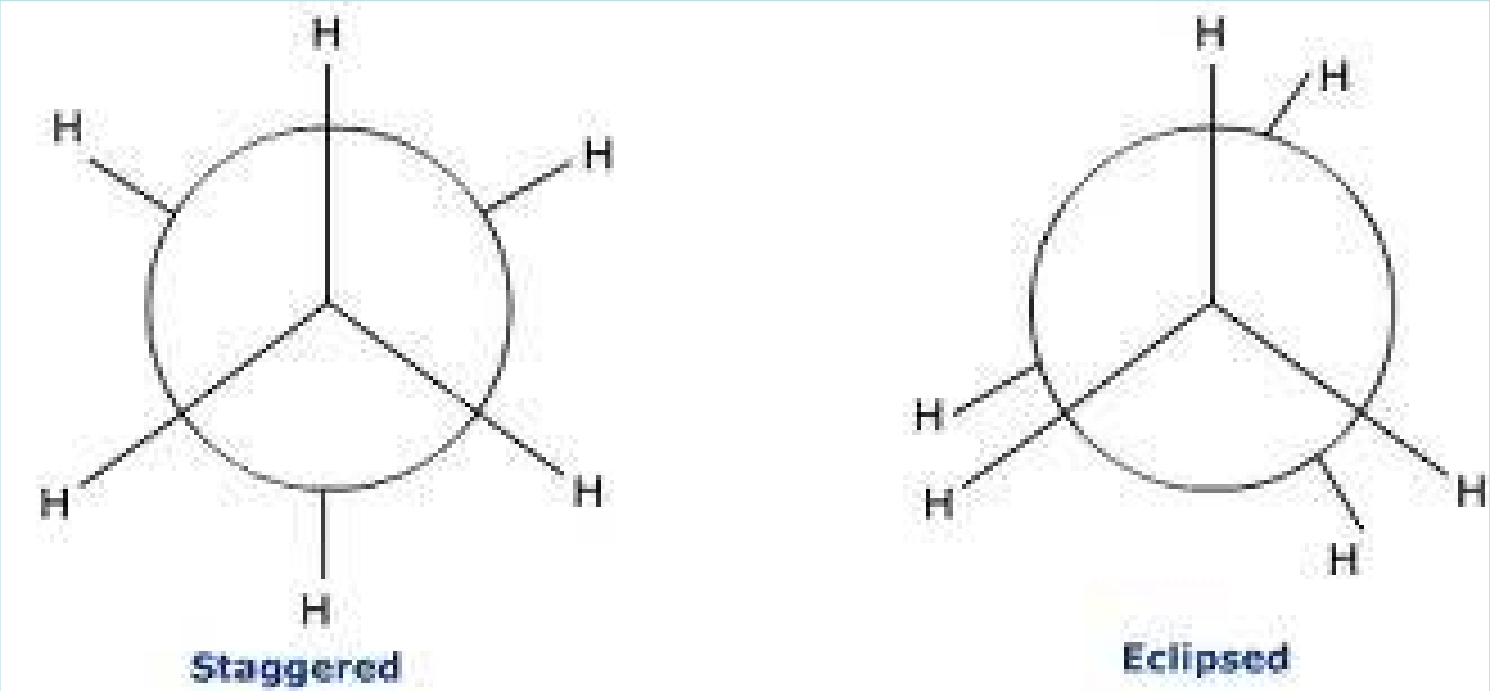
Ethane



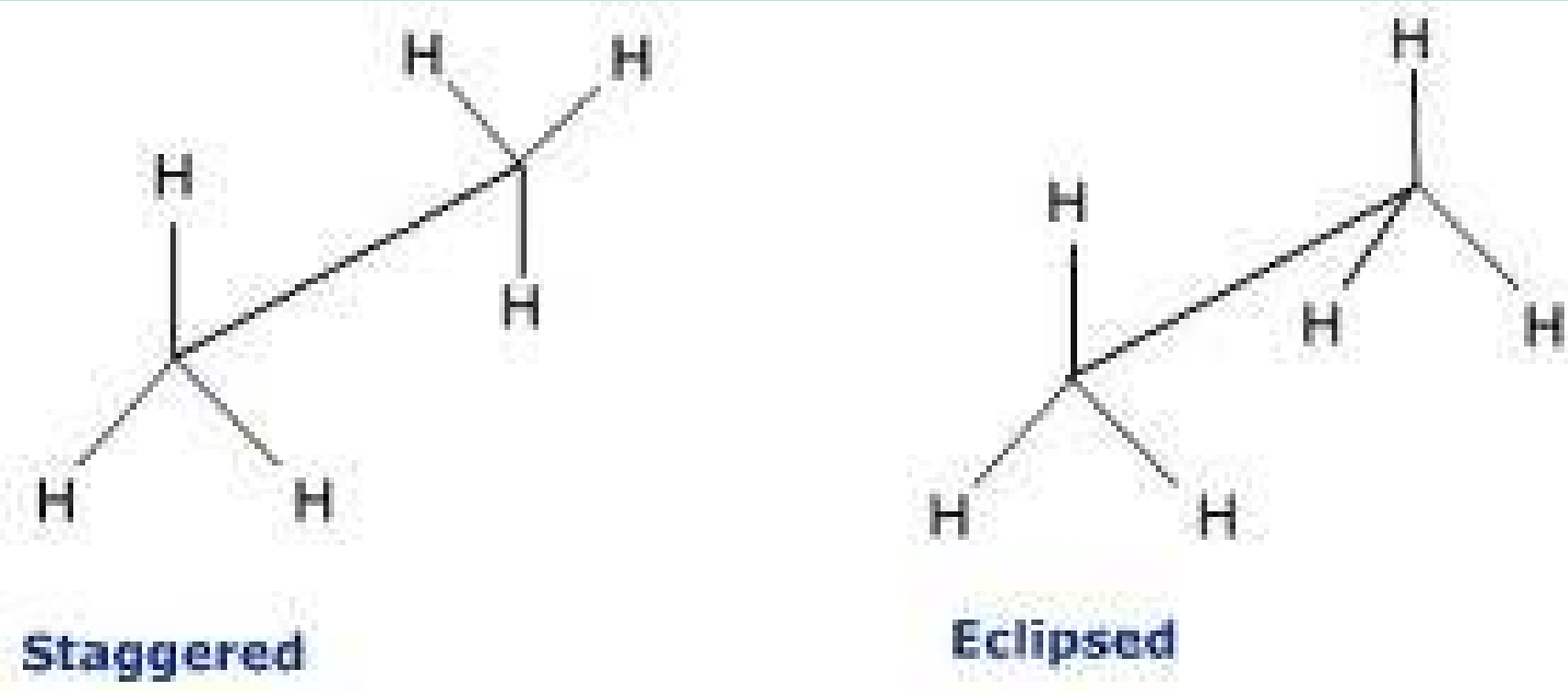


- staggered conformation

Newman Projection

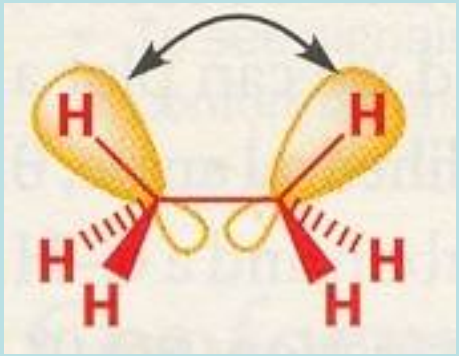


Sawhorse Projection

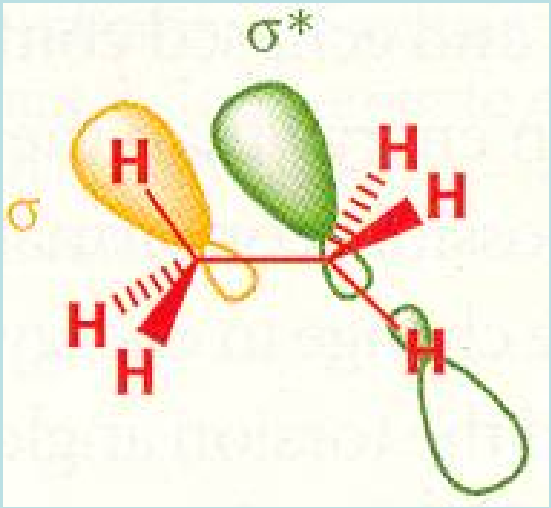


Torsional strain

Caused by repulsion of the bonding electrons of one substituent with the bonding electrons of a nearby substituent



filled orbitals repel

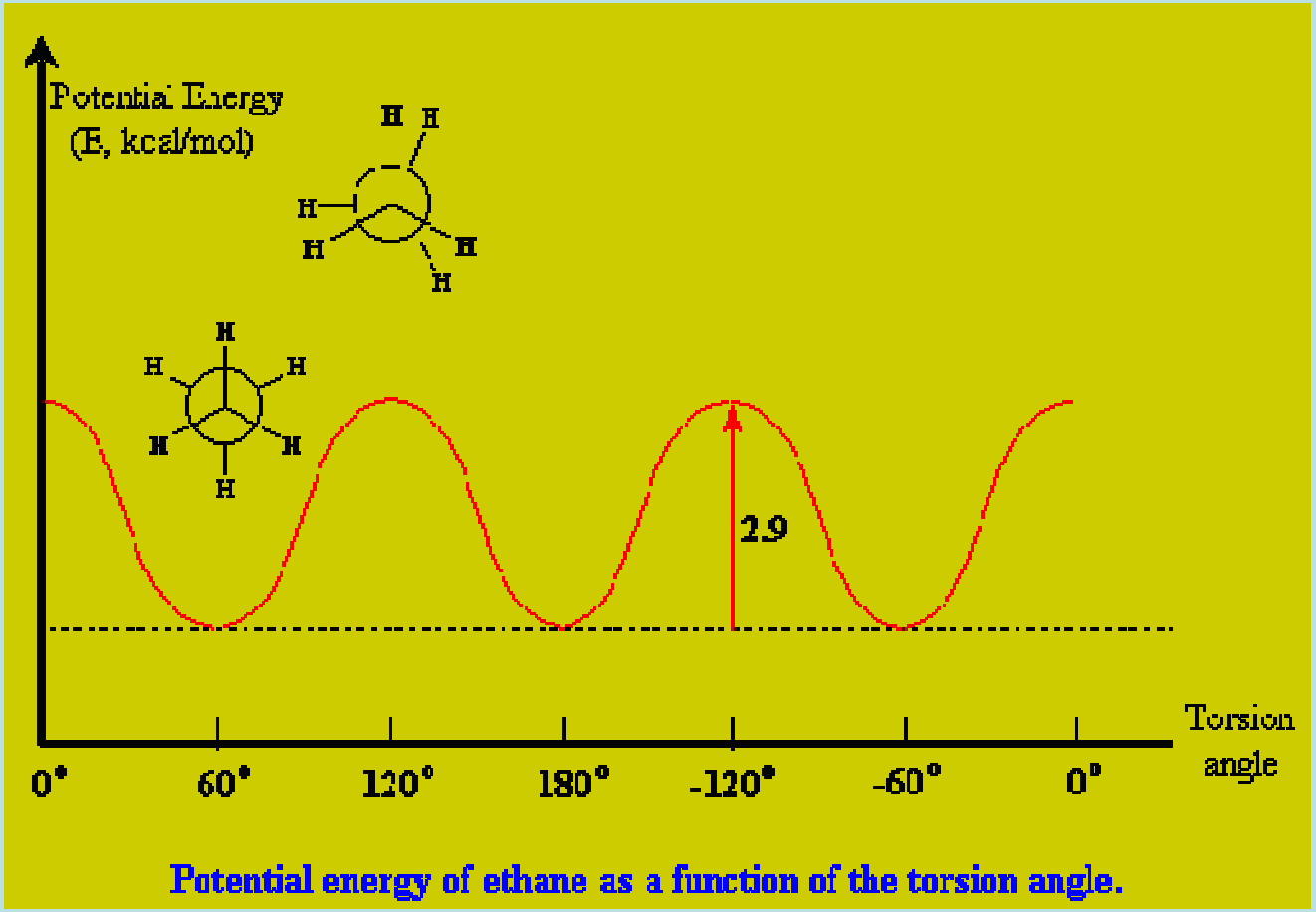


- Stabilizing interaction between filled C-H σ bond and empty C-H σ^* antibonding bonding orbital

The real picture is probably a mixture of all 3 effects

- **The rotational barrier is (12 kJ/mol) small enough to allow the conformational isomers to interconvert million of times per second**

Potential energy of ethane as function of torsion angles



Potential energy of ethane as a function of the torsion angle.

- staggered conformation has potential energy minimum
- eclipsed conformation has potential energy maximum
- staggered conformation is lower in energy than the eclipsed by 2.9 kcal/mole (12 kJ/mole)

References:

1. Advanced Organic Chemistry By Carey and Sundberg, Cahpter 3 , Part- A
2. Advanced Stereochemistry by D. Nasipuri
3. Advanced Stereochemistry by S Sengupta
4. Advanced Stereochemistry by Eliel.