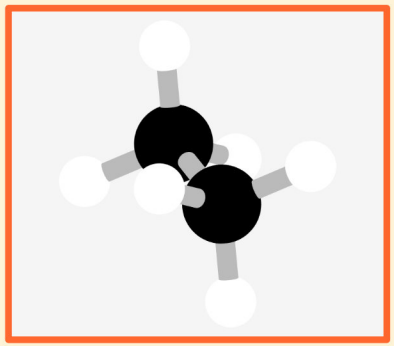
# HIGHLIGHTS

- Rotation of σ bonds allowed but π bonds cannot rotate
- Different conformations can be represented by skeletal, sawhorse and Newman projections
- Ethane has two conformations
- Butane has four conformations



Single or σ bonds are free to rotate. Multiple bonds, those with π bonds cannot. When a single bond rotates, the shape of the molecule changes. The different shapes are known as ***conformations***. Some conformations are more favorable or stable than others. These are known as ***conformers***. Other shapes are disfavored, these slow rotation and are ***barriers to rotation***. It is possible to represent the different conformations in drawings using skeletal, sawhorse and Newman projections. This summary introduces the conformations of simple molecules.





CHEMISTRY CLASSICS

# CONFORMATIONS OF ALKANES

## SIMPLE ACYCLIC ALKANES

# Conformations of simple alkanes

## 1. Which bonds rotate?

*view from side of alkane* — rotate — *view along bond* — rotate

*view from side of alkene* — rotate — *view along bond* — rotate

Rotation of a σ bond is allowed as it doesn't disrupt overlap of the 2 bonding orbitals.
Rotation of a π bond is ***not*** allowed as it breaks the overlap of the 2p orbitals.

## 2. Representing conformations

**skeletal** *representation*

pull rhs carbon forward & down

**sawhorse** *representation*

nudge front atom right & down to reveal C–C bond

**Newman** *projection*

**Line drawing to Newman projection**

1. eye is **blue** arrow looking along **C–C** draw dot • representing first C
2. **H** is vertical - draw upwards from dot
3. **F** to right of eye (looking along →)
4. **$CH_3$** opposite corner of triangle
5. move to back atom - draw **big circle**
6. **H** same side as **F**
7. **HO** same side as **$CH_3$**
8. final $CH_3$ vertical down

## 3. The conformations of ethane

**staggered**
Favored conformation
A *conformer*

**eclipsed**
Disfavored (torsional strain)
*Barrier to rotation*

maximum repulsion

favourable interaction

**torsional strain**
Repulsion between bonds
**hyperconjugation**
Stabilizes staggered

## 4. The conformations of butane

**antiperiplanar**
*most favoured*
no strain

**anticlinal**
disfavoured
torsional strain

**synclinal (gauche)**
favoured
steric strain

**synperiplanar**
*most disfavoured*
torsional & steric

**Steric strain** - repulsion between atoms, causes the *gauche* (staggered) conformer (local energy minima) to be higher in energy than the *antiperiplanar* conformer. The *synperiplanar* (eclipsed) conformation is the *barrier to rotation* or a *transition state*.

## 5. Conformations of larger molecules

draw most & least favoured conformation along this bond →

current conformation

largest substituents antiperiplanar (staggered) **favoured**

largest substituents eclipsed **disfavoured**