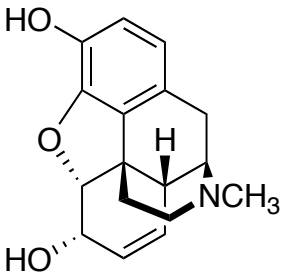
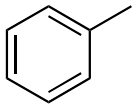
Conformational Analysis
the shape of organic molecules

shape controls activity

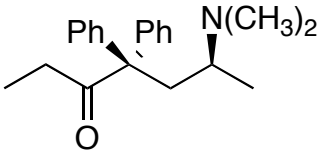
morphine
an addictive analgetic



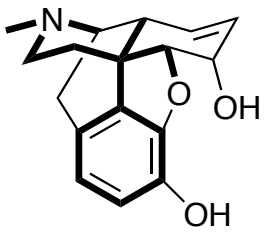


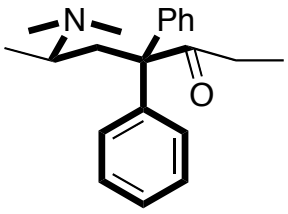
= Ph

methadone
as potent as morphine,
but non-addictive



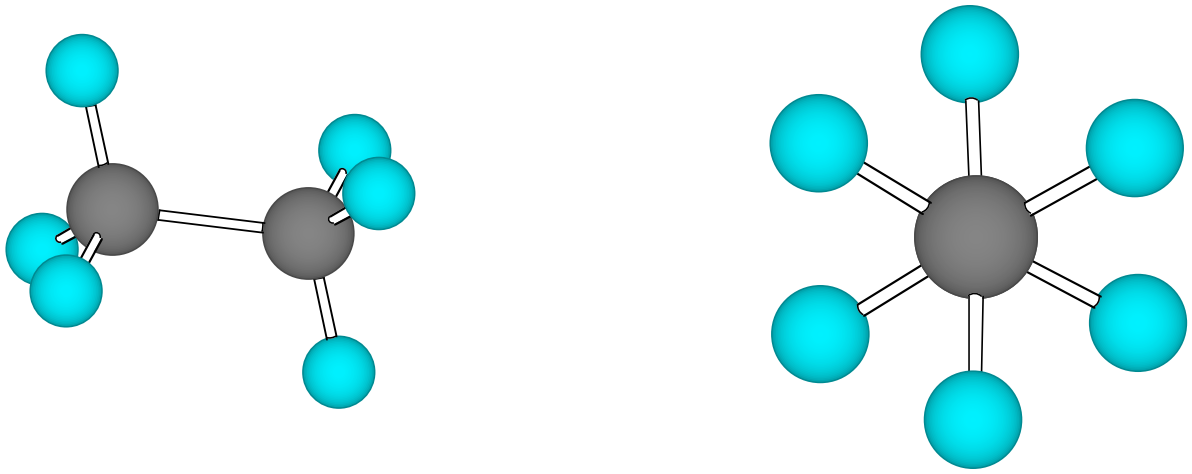
these molecules bind to the same receptor in the brain because they have similar shape



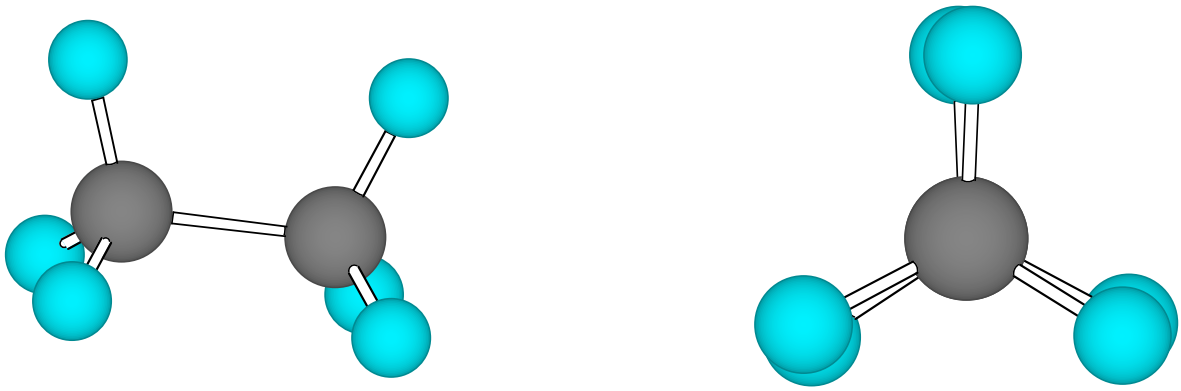


Conformational Isomers (Conformers) of Ethane

Staggered: the dihedral angle between hydrogens on adjacent carbons is 60˚ (or 180˚).



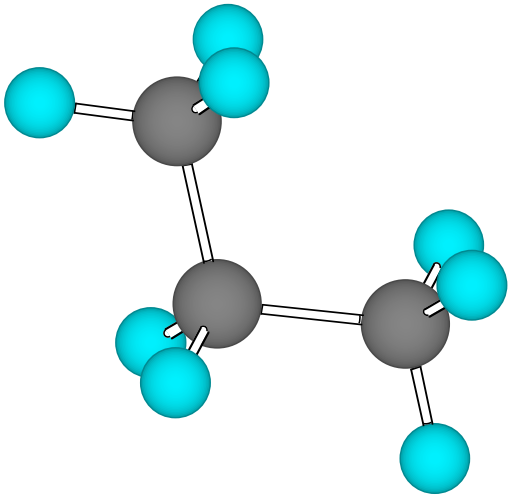
Eclipsed: the dihedral angle between hydrogens on adjacent carbons is 0˚.

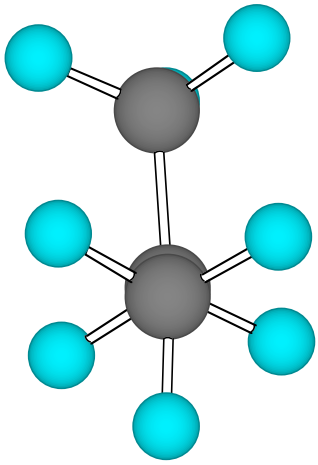


The **staggered** conformer of ethane is more stable than the **eclipsed** conformer by about 3 kcal/mol (1 kcal/mol for each **eclipsing interaction**).

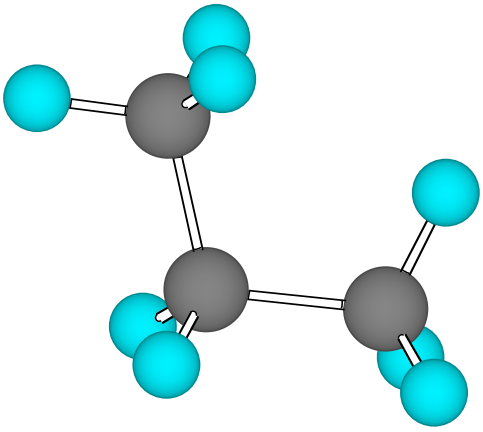
Conformational Isomers (Conformers) of Propane
–similar to ethane–

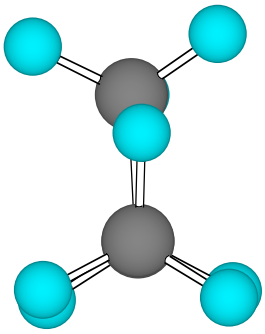
Staggered: the dihedral angle is 60˚ (or 180˚).





Eclipsed: the dihedral angle is 0˚.

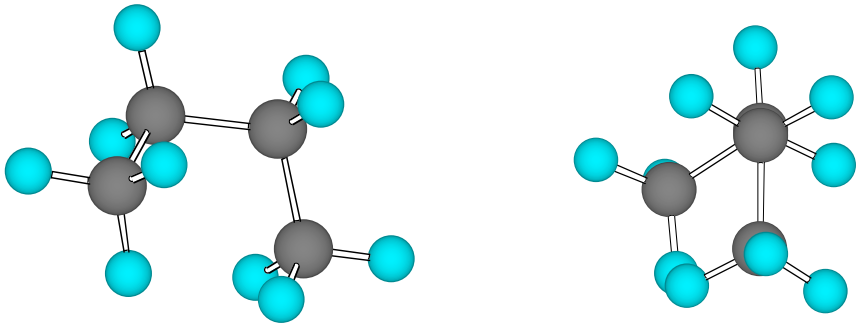




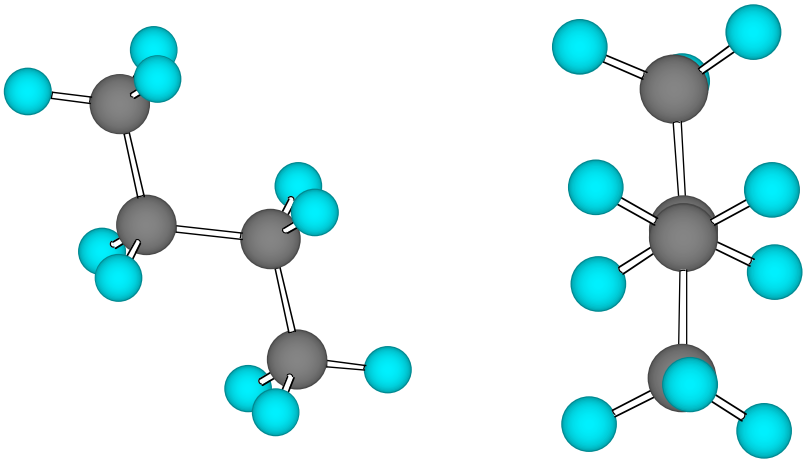
The **staggered** conformer of propane is more stable than the **eclipsed** conformer by about 3.4 kcal/mol

Staggered Isomers of Butane

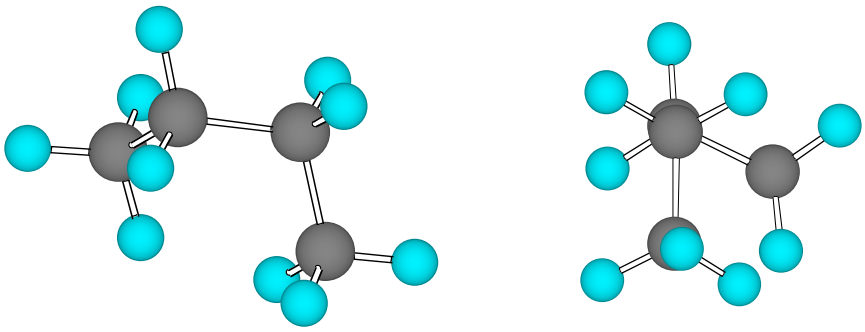
Gauche: the Me/Me dihedral angle is –60˚



Antiperiplanar: the Me/Me dihedral angle is 180˚.



Gauche: the Me/Me dihedral angle is +60˚



The **antiperiplanar** conformer of butane is more stable than the **gauche** conformers by about 0.9 kcal/mol