

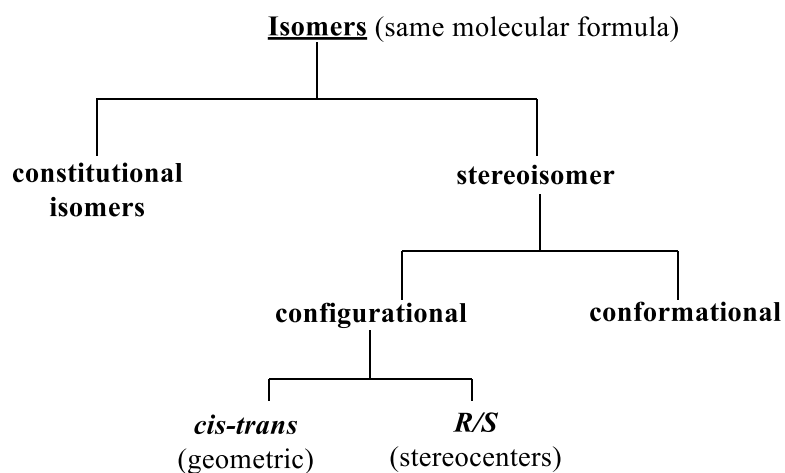
Ch 4 Alkanes and Cycloalkanes

I. Nomenclature

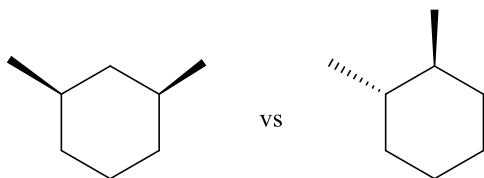
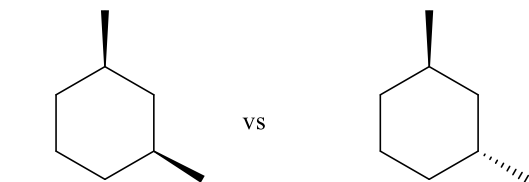
- a. IUPAC rules
- b. handout
 - i. find parent chain
 - ii. name substituents
 - iii. assign number locant to substituents (keep numbers as low as possible)
 - iv. alphabetize substituents

stereo – substituents – parent – unsaturation – functional group

II. Constitutional isomers

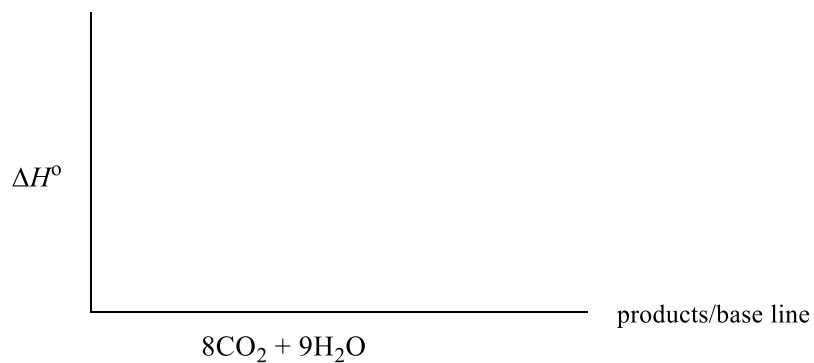
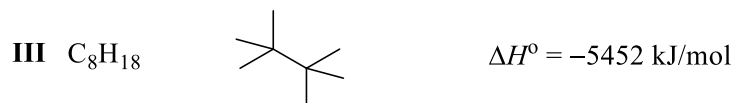
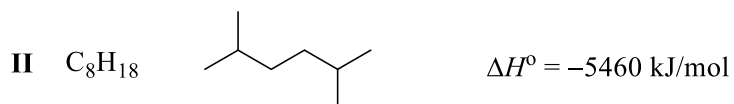
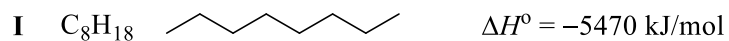


Constitutional isomers have _____



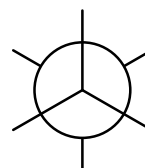
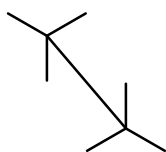
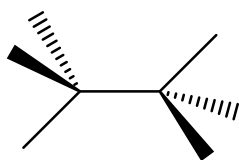
Relative stabilities of alkanes are determined by combustion

branched alkanes are _____ stable than straight-chain alkanes



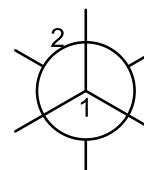
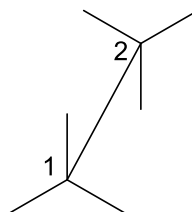
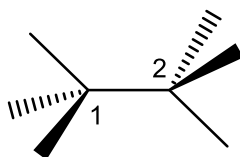
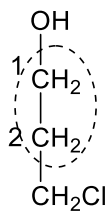
III. Newman projections

a. convert: wedge and dash \rightarrow sawhorse \rightarrow Newman projection, and vice versa

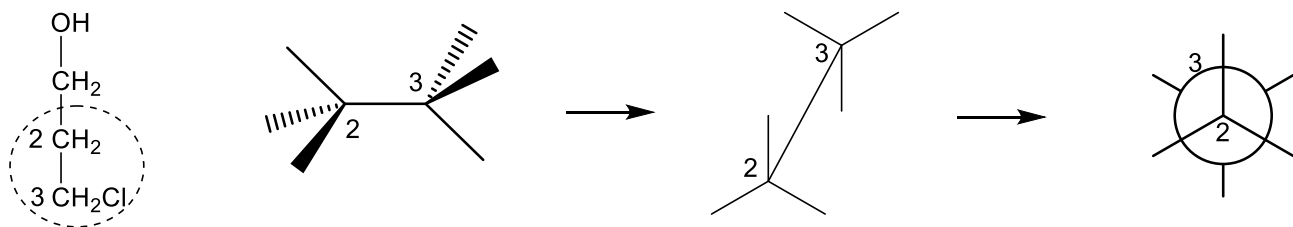


Let's take a look at 3-chloropropan-1-ol

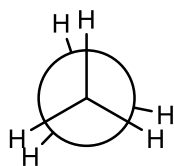
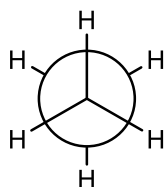
look down C-1 to C-2



look down C-2 to C-3



Conformations of ethane



The angle between the H-atoms is called the _____ or _____.

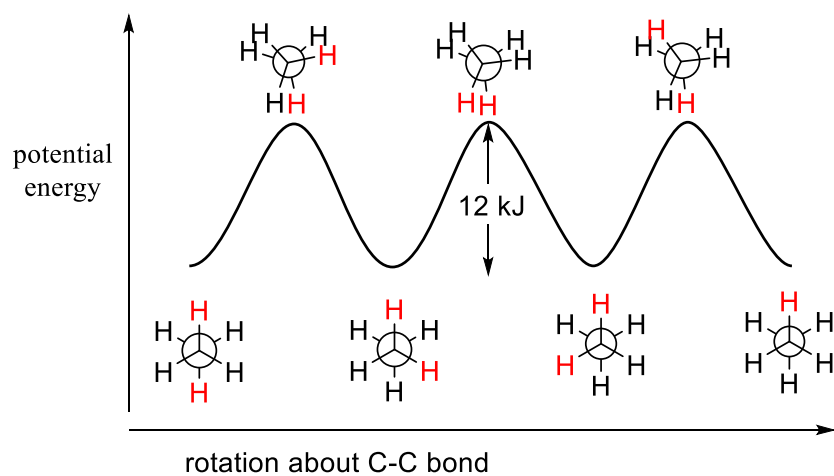
IV. Conformational analysis

a. Terms

- i. staggered
- ii. eclipsed
- iii. anti-periplanar
- iv. gauche

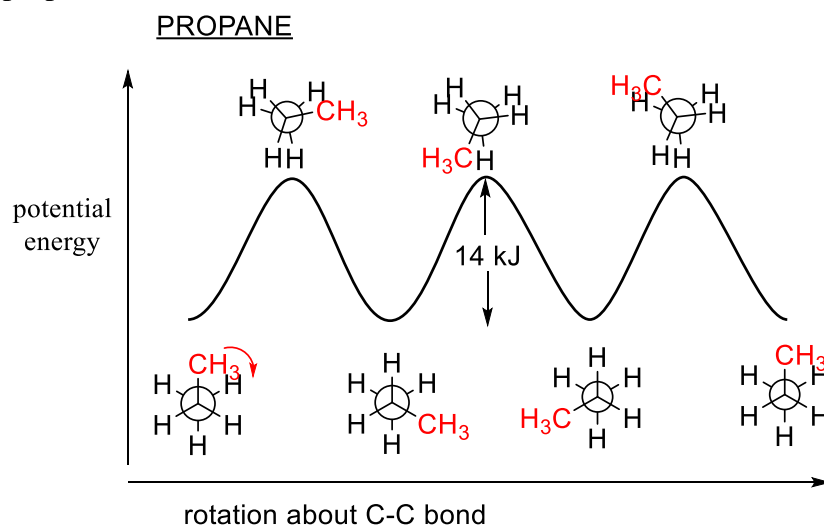
b. ethane

ETHANE

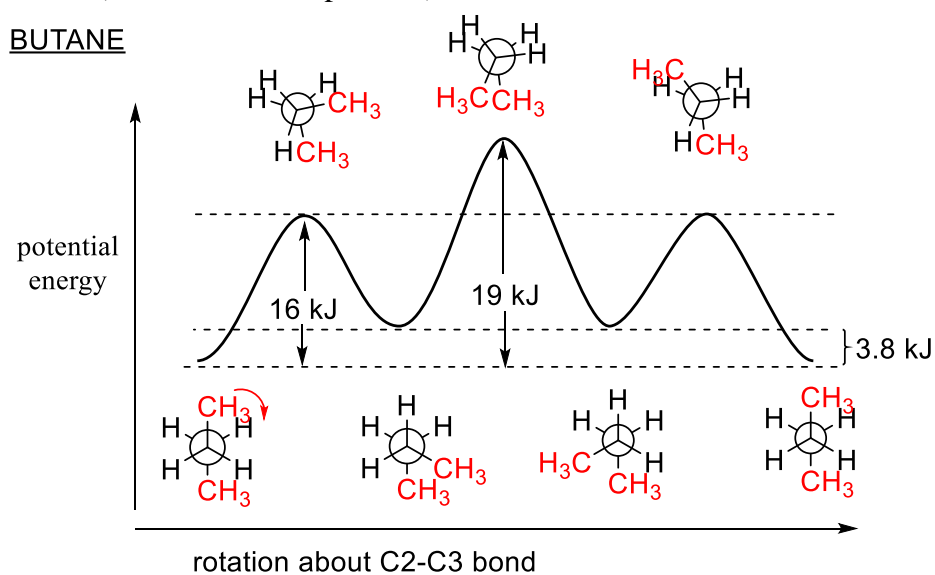


we are rotating the front carbon and holding the carbon in the back steady

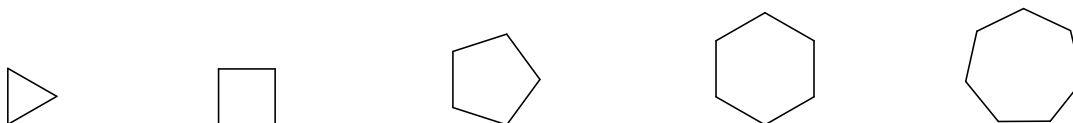
c. propane



d. butane (a little more complicated)

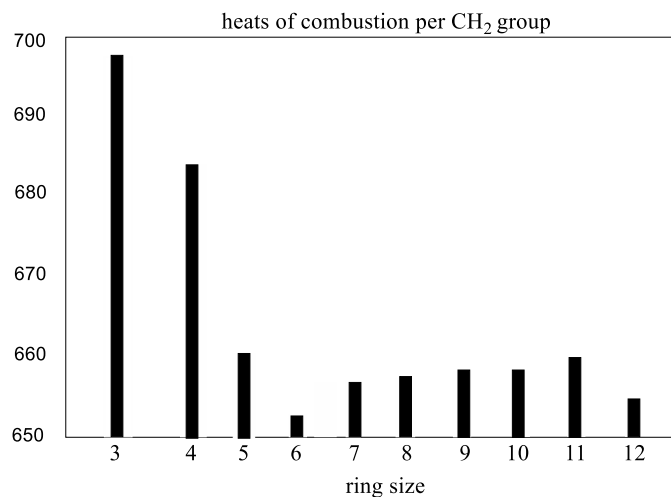


V. Cycloalkanes

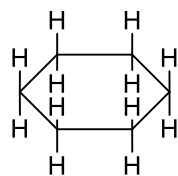


all of the above contain sp^3 carbons

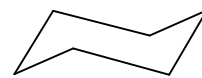
ring strain is a combination of torsional strain (dihedral angle) and angle strain



So why does cyclohexane appear to be the most stable?



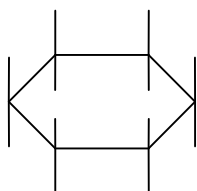
flat



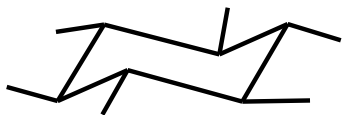
puckered

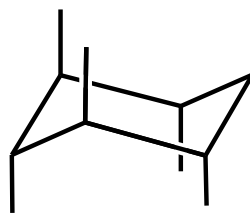
VI. Conformations of cyclohexane

- Cyclohexane can twist into other shapes but the chair is always most stable/lowest energy
- *cis* and *trans* stereoisomers of cyclohexane



a. axial and equatorial positions

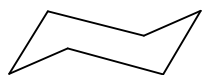




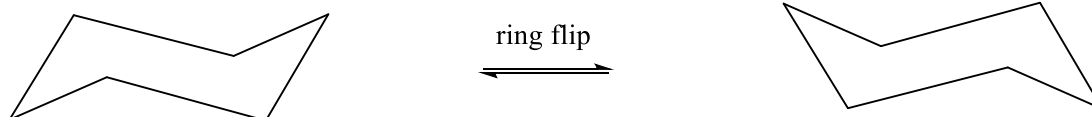
b. stability of chair conformations

bulky groups are more stable in equatorial position, *if possible*

i. 1,3-diaxial interactions



ii. monosubstituted



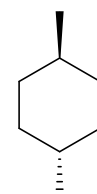
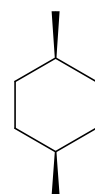
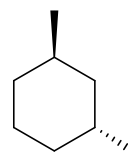
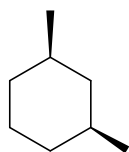
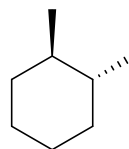
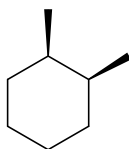
iii. disubstituted

1, 2

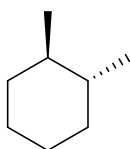
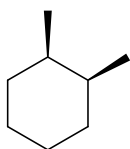
1, 3

1, 4

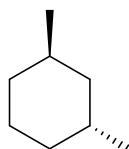
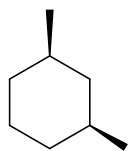
cis and trans



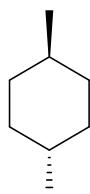
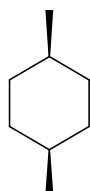
let's do 1,2



let's do 1,3 – *cis* and *trans*



let's do 1,4 – *cis* and *trans*



Summary for disubstituted cyclohexane

1,2 – *cis* : *a,e* or *a,e* equal

1,2 – *trans* : *a,a* or *e,e*

1,3 – *cis* : *a,a* or *e,e*

1,3 – *trans* : *e,a* or *a,e* equal

1,4 – *cis* : *a,e* or *e,a* equal

1,4 – *trans* : *a,a* or *e,e*

iv. polysubstituted

the bulkiest group should be equatorial, usually

	1,3-diaxial energy	<i>e:a</i> ratio
-Cl	2.0 kJ/mol	70:30
-OH	4.2	83:17
-CH ₃ (Me)	7.6	95:5
-CH ₂ CH ₃ (Et)	8.0	96:4
-CH(CH ₃) ₂ (<i>i</i> -Pr)	9.2	97:3
-C(CH ₃) ₃ (<i>t</i> -Bu)	22.8	9999:1

v. polycyclics – *cis* and *trans* decalin

consider the H-atoms on two fused C-atoms

