Chapter 3: Structure and Stereochemistry of Alkanes

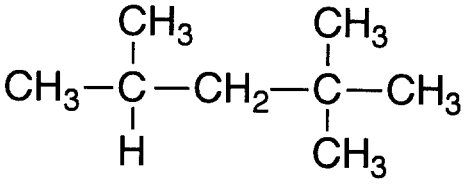
HYDROCARBONS

saturated
- maximum number of hydrogens
- all single bonds
- alkanes/cycloalkanes

unsaturated
- π bonds
- alkenes/alkynes/aromatic

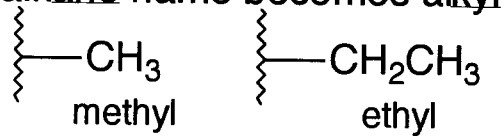
Table 3-2, page 81: Know the names of the first ten alkanes!

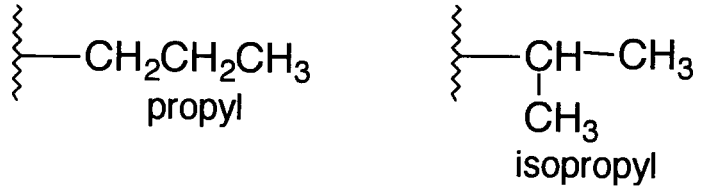
Classification of Carbons and Hydrogens:

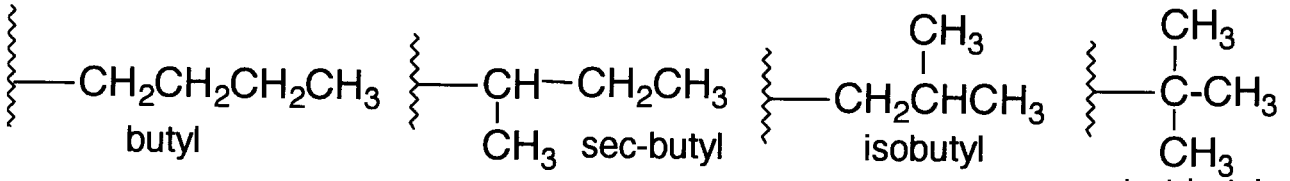


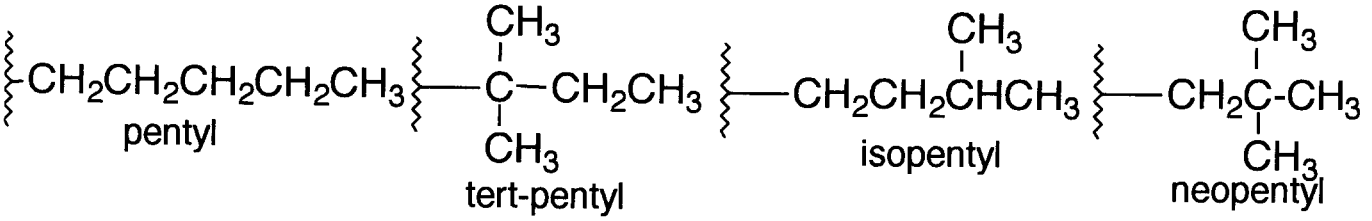
Naming alkyl groups/side chains (common names included):

- alkane name becomes alkyl name



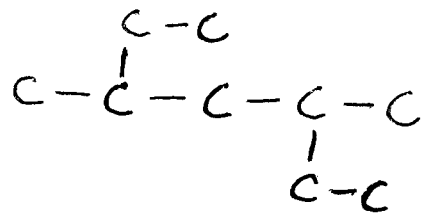




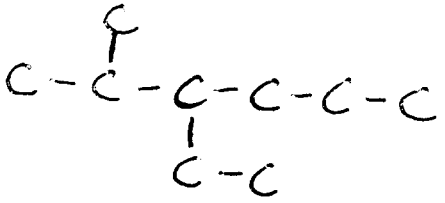


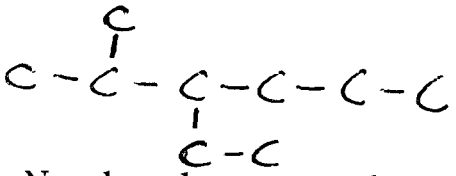
IUPAC Rules : Prefix-Parent-Suffix

1. Find longest continuous carbon chain. Make that chain the parent.

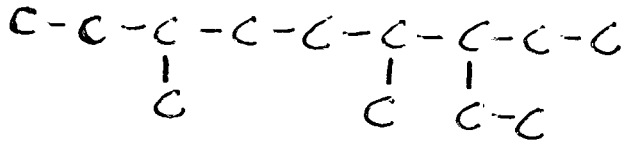


If two different chains of equal length are possible, choose as the parent the one with the most substituents.



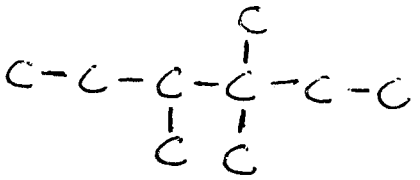


2. Number the parent chain to give the substituents the lowest possible set of numbers. (Use first point of difference rule to determine which is the lowest set.)

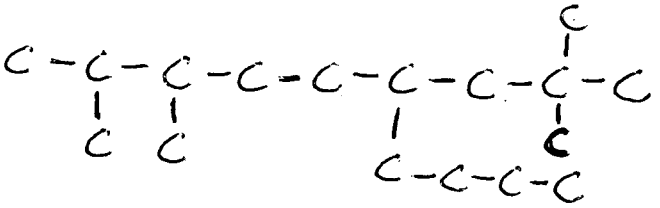


3. Identify and number each substituent.

4. Write the name as a single word:
   a. use hyphens to seperate substituents from numbers
   b. use commas to seperate numbers
   c. use Greek prefixes (di, tri, tetra, etc.) to indicate number when more than one of any type of substituent is present
   d. write substituents in alphabetical order (ignore di ,tri, etc., and sec.-, tert.-, but "iso" and "neo" count)

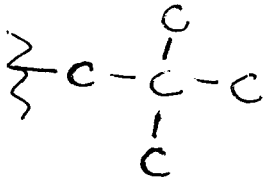


5. Naming a complex side chain (substituent):



   a. If it has an accepted common name, use it!

   b. Name it according to previous rules.
      1. Find longest chain for parent name.
      2. Number that chain beginning with point of attachment to main chain.
      3. Name and number substituents.
      4. Place complex substituent name in parentheses.



Physical Properties:

1. Solubility:

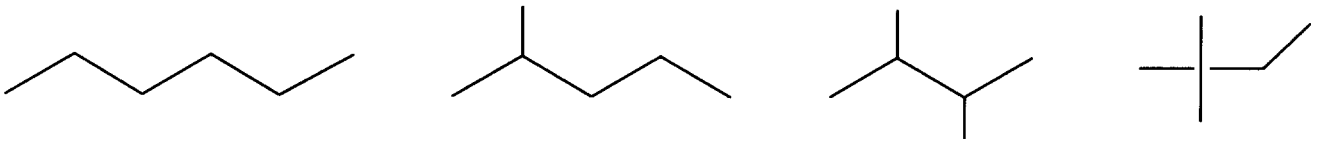
2. Density:

3. Boiling Point: (Ch. 2) greater the surface area (MW), greater the BP
branching decreases surface area, so decreases BP

4. Melting Point: (Fig. 3-4, p. 89) In general, greater the MW, greater theMP,
but increase is not steady.

Crystal Packing:

Branching:



Reactions of Alkanes:

1. Combustion (oxidation)

$$\text{alkane} + O_2 \xrightarrow{\text{heat}} CO_2 + H_2O$$

2. Cracking and Hydrocracking

$$\text{large hydrocarbons} \xrightarrow{\text{heat}} \text{smaller hydrocarbons}$$

3.Halogenation (Chapter 4) - a free radical substitution

$$CH_4 + Cl_2 \xrightarrow[\text{or light}]{\text{heat}} CH_3Cl + HCl + \text{others}$$

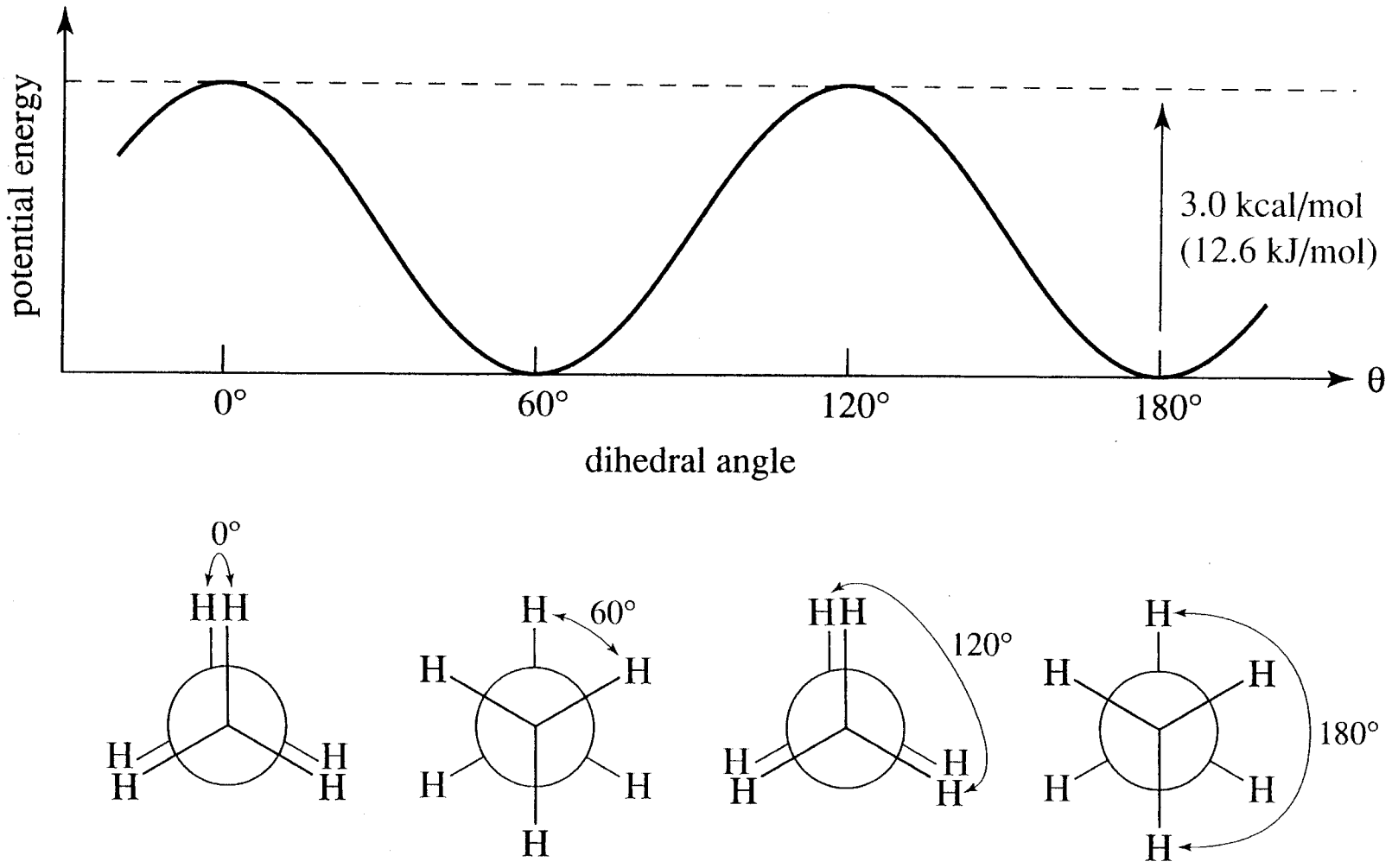
Structure and Conformations of Alkanes

conformations - temporary arrangements of atoms that result from rotation around single bonds

Newman Projections:

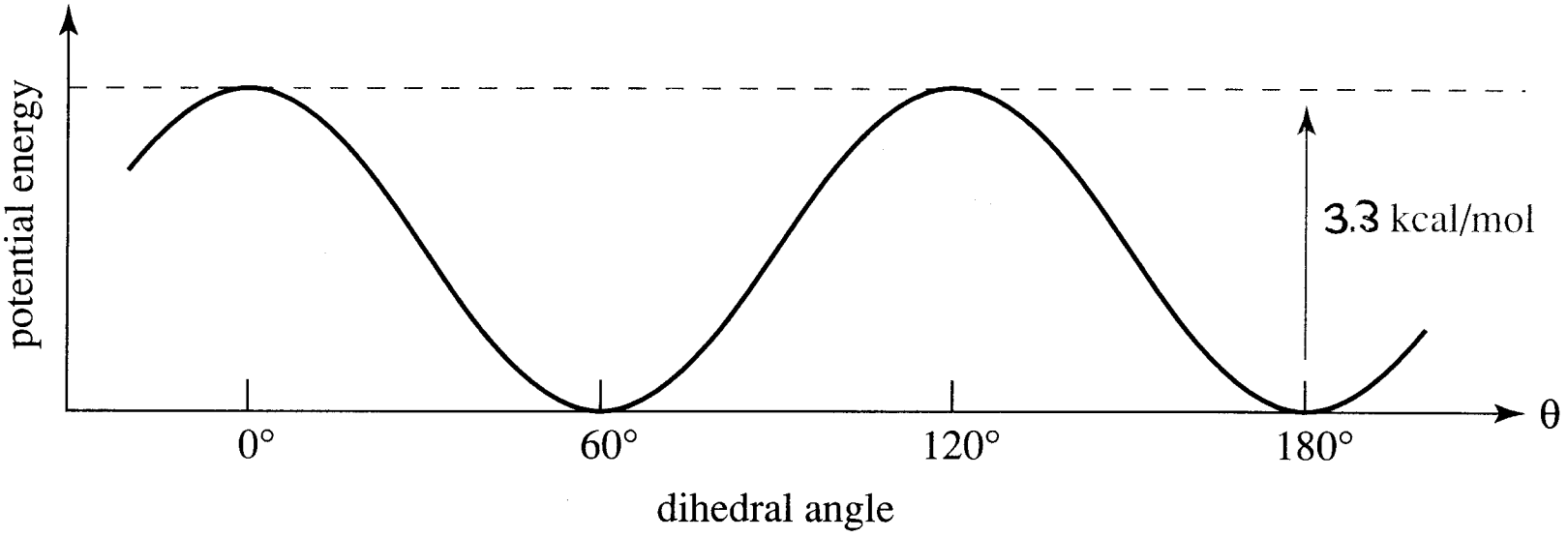
T-16

Fig. 3-7 Torsional Energy of Ethane



view → CH_2CH_3 (with CH_3 below)

Torsional Energy of Propane



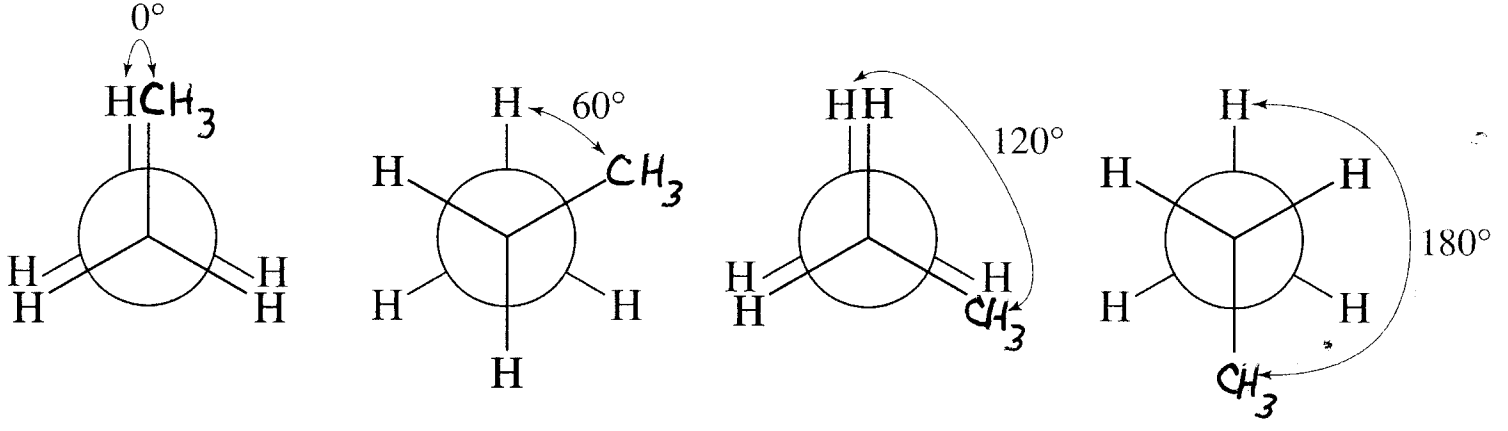
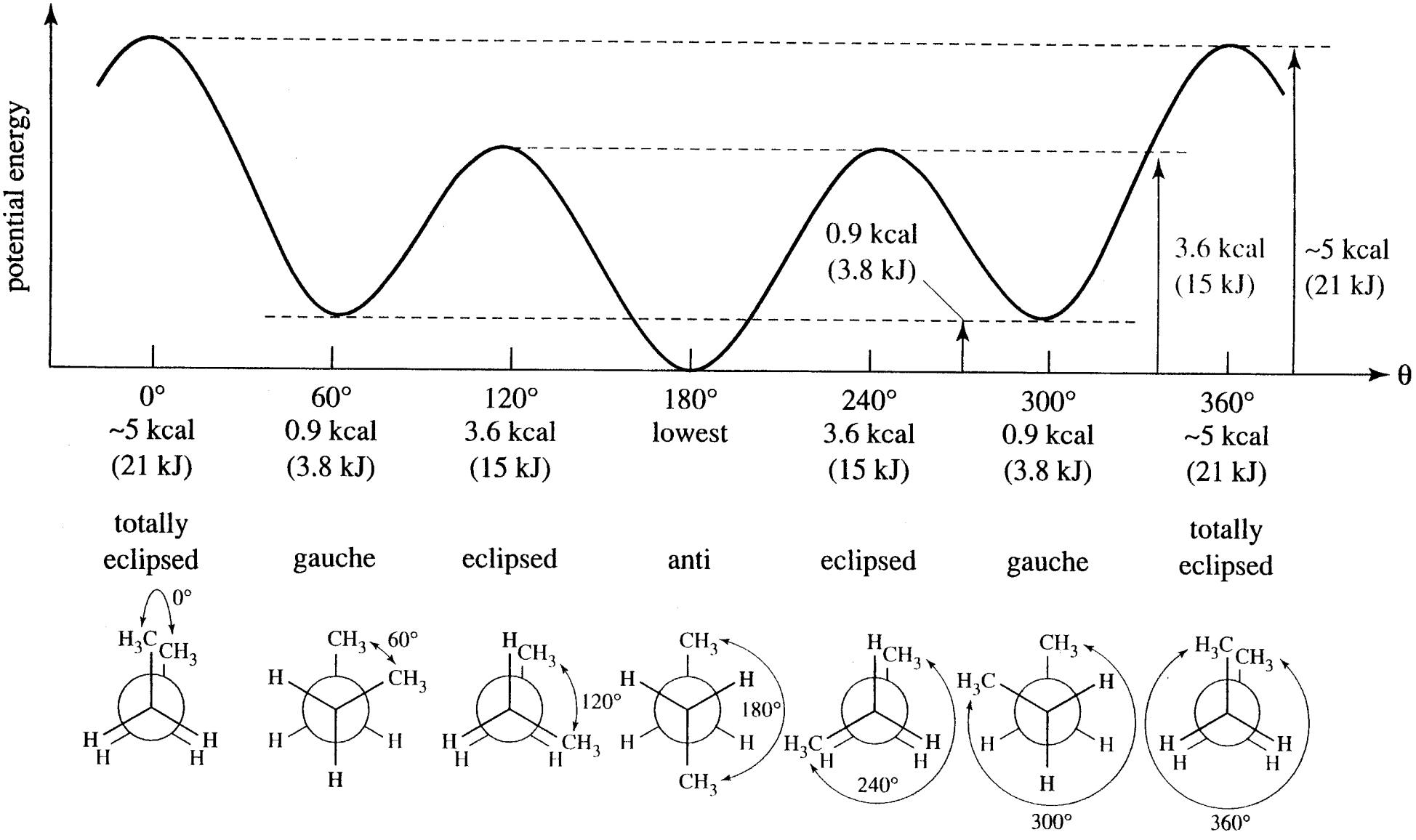


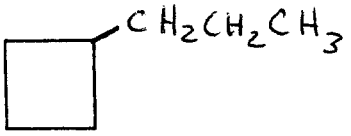
Fig. 3-11 Torsional Energy of Butane

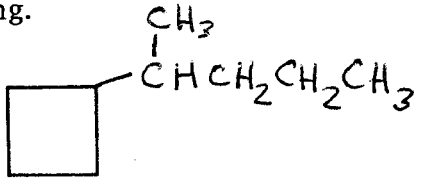


IUPAC RULES: Cycloalkanes

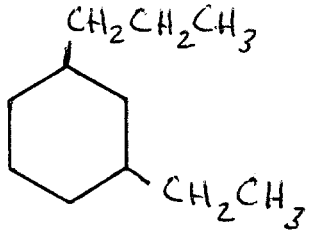
1. For unsubstituted cycloalkanes, add "cyclo" to the alkane name of the same carbon number.

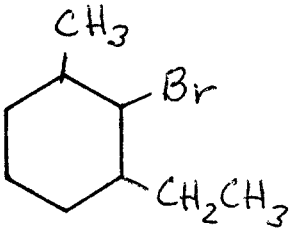
2. For substituted cycloalkanes, use the cycloalkane name as the parent name unless a side chain has more carbon atoms than the ring.





3. Number the substituents to give the lowest possible numbers. (First point of difference) If the set of numbers obtained is the same from two numbering directions, use alphabetical priority to decide the substituent numbers. (Alphabetical priority is sometimes necessary in acyclic alkanes.)





4. Indicate stereochemistry when necessary (cis/trans or R/S).

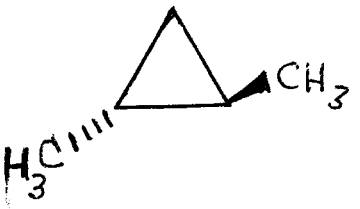


Fig. 3-15 Angle Strain in Cyclopropane

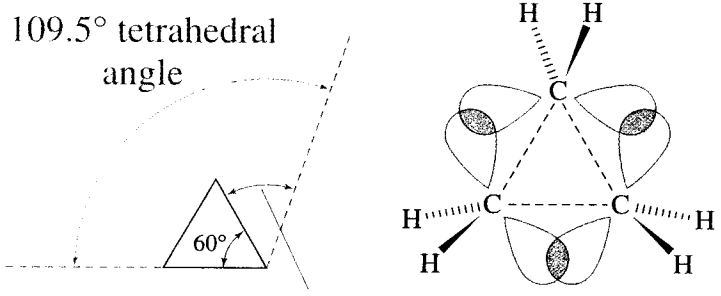
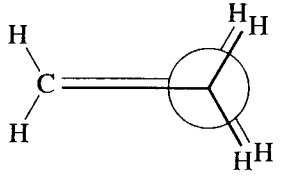


Fig. 3-16 Torsional Strain in Cyclopropane



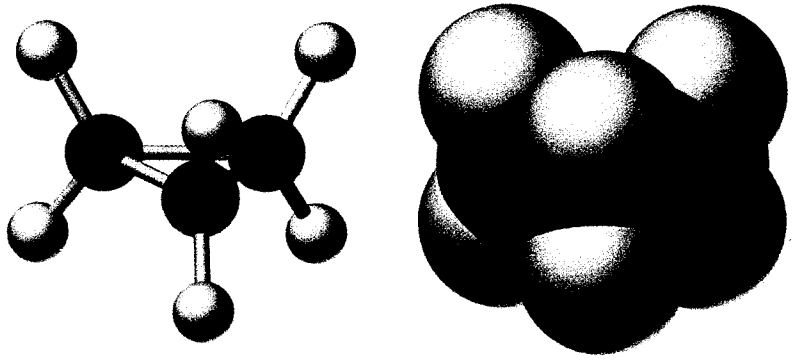


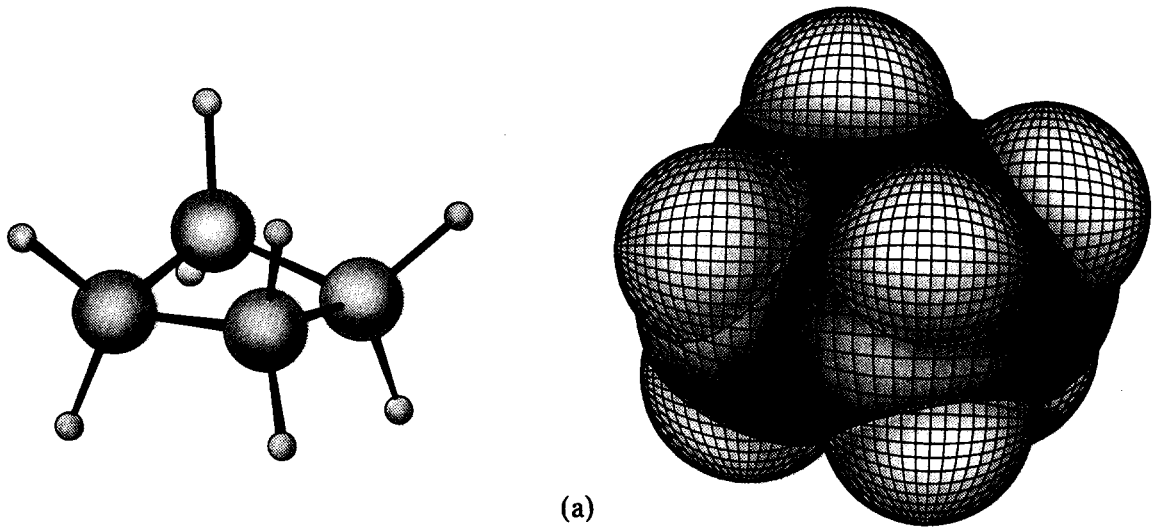
Table 3-4

TABLE 3-4 Heats of Combustion (Per Mole) for Some Simple Cycloalkanes

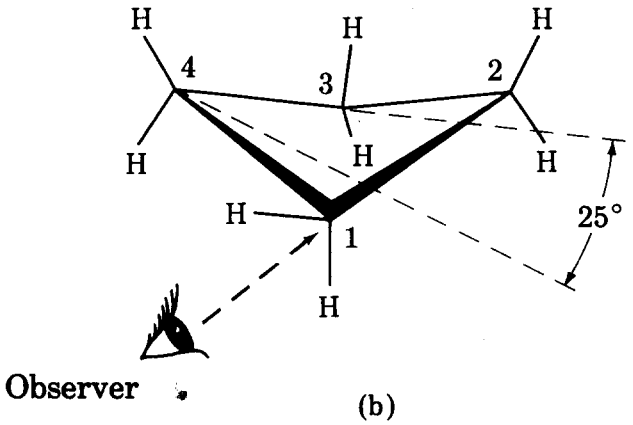
Ring size	*Cycloalkane*	*Molar Heat of Combustion*	*Heat of Combustion per CH_2 Group*	*Ring Strain per CH_2 Group*	*Total Ring Strain*
3	cyclopropane	499.8 kcal	166.6 kcal	9.2 kcal	27.6 kcal (115 kJ)
4	cyclobutane	655.9 kcal	164.0 kcal	6.6 kcal	26.4 kcal (110 kJ)
5	cyclopentane	793.5 kcal	158.7 kcal	1.3 kcal	6.5 kcal (27 kJ)
6	cyclohexane	944.5 kcal	157.4 kcal	0.0 kcal	0.0 kcal (0.0 kJ)
7	cycloheptane	1108.3 kcal	158.3 kcal	0.9 kcal	6.3 kcal (26 kJ)
8	cyclooctane	1268.9 kcal	158.6 kcal	1.2 kcal	9.6 kcal (40 kJ)
reference: long-chain alkane			157.4 kcal	0.0 kcal	0.0 kcal (0.0 kJ)

Transparency 18 *Figure* 4.11 *Page* 116

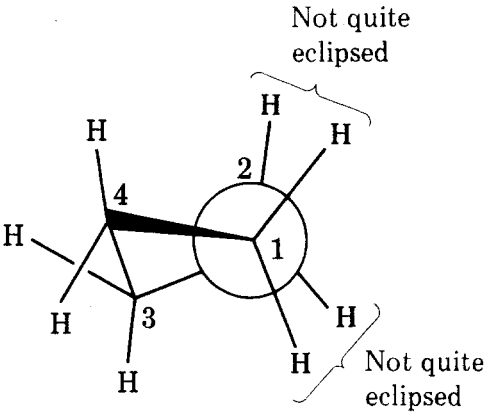
Conformation of cyclobutane



(a)



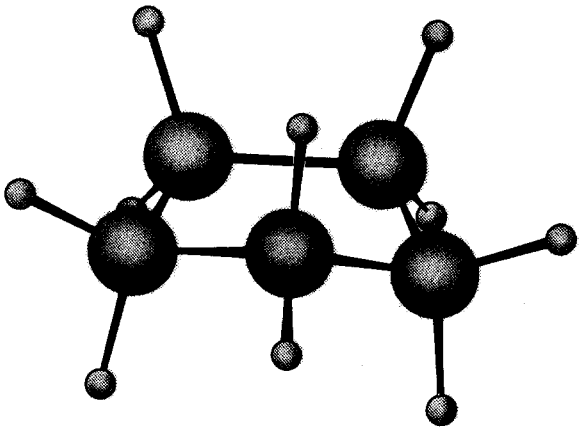
(b)

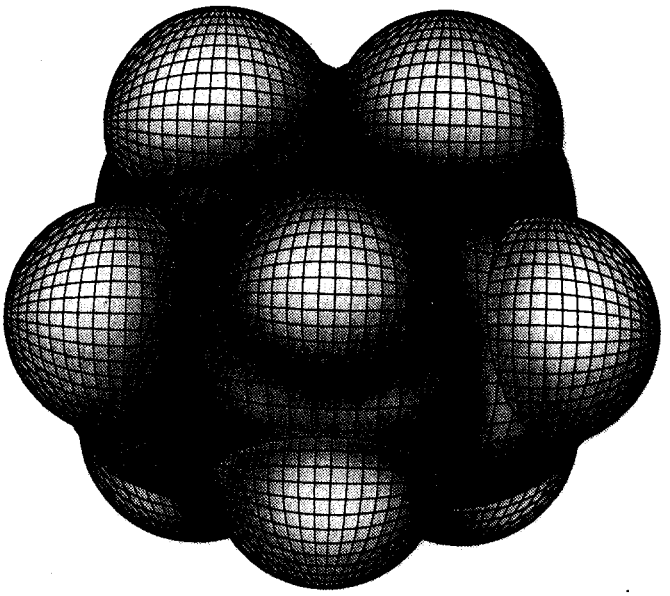


(c)

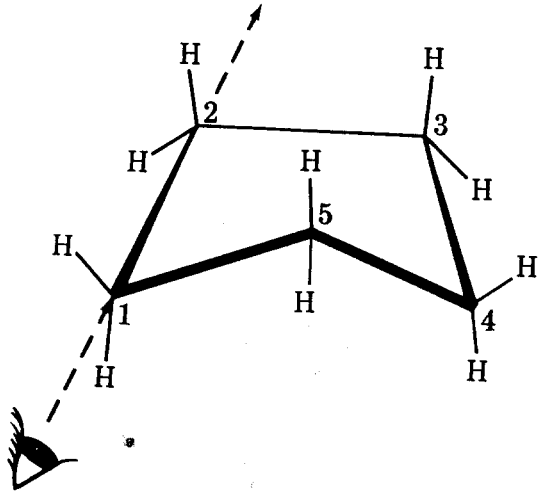
Transparency 19 *Figure* 4.12 *Page* 117

Conformation of cyclopentane



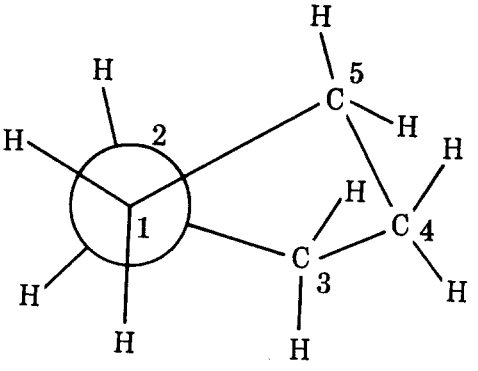


(a)



Observer

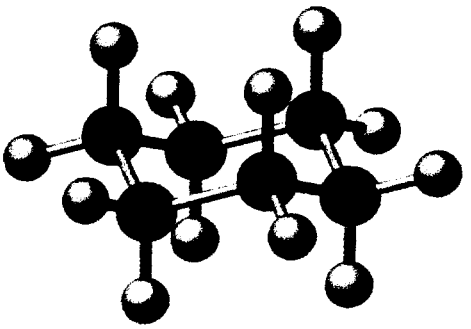
(b)



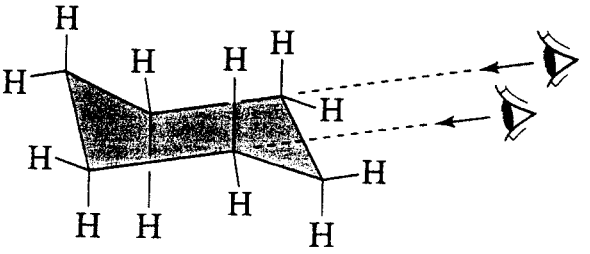
(c)

T-20

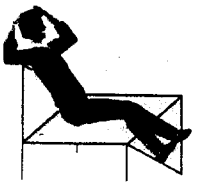
Fig. 3-19 Cyclohexane Chair Conformation

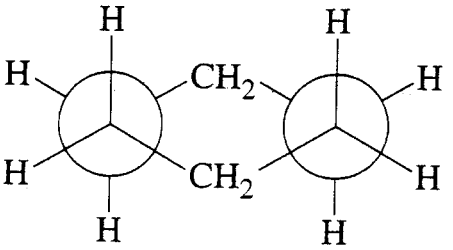


chair conformation of cyclohexane



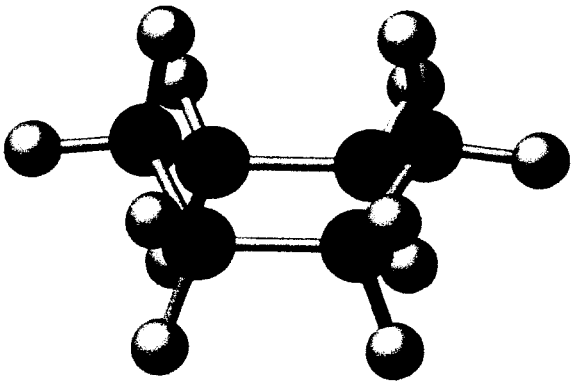
chair conformation



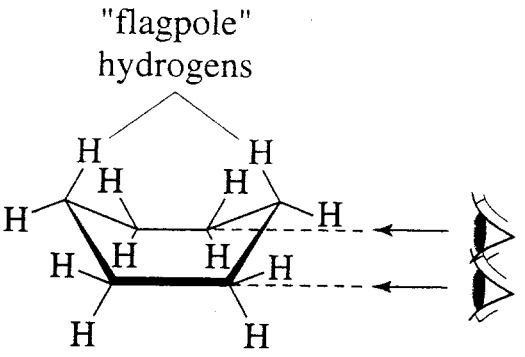


Newman projection

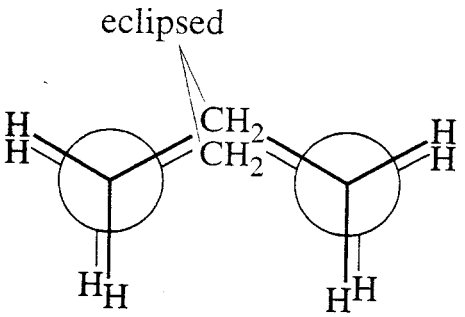
Fig. 3-20 Cyclohexane Boat Conformation



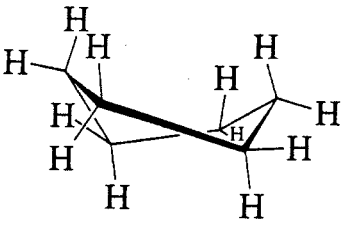
boat conformation of cyclohexane



symmetrical boat



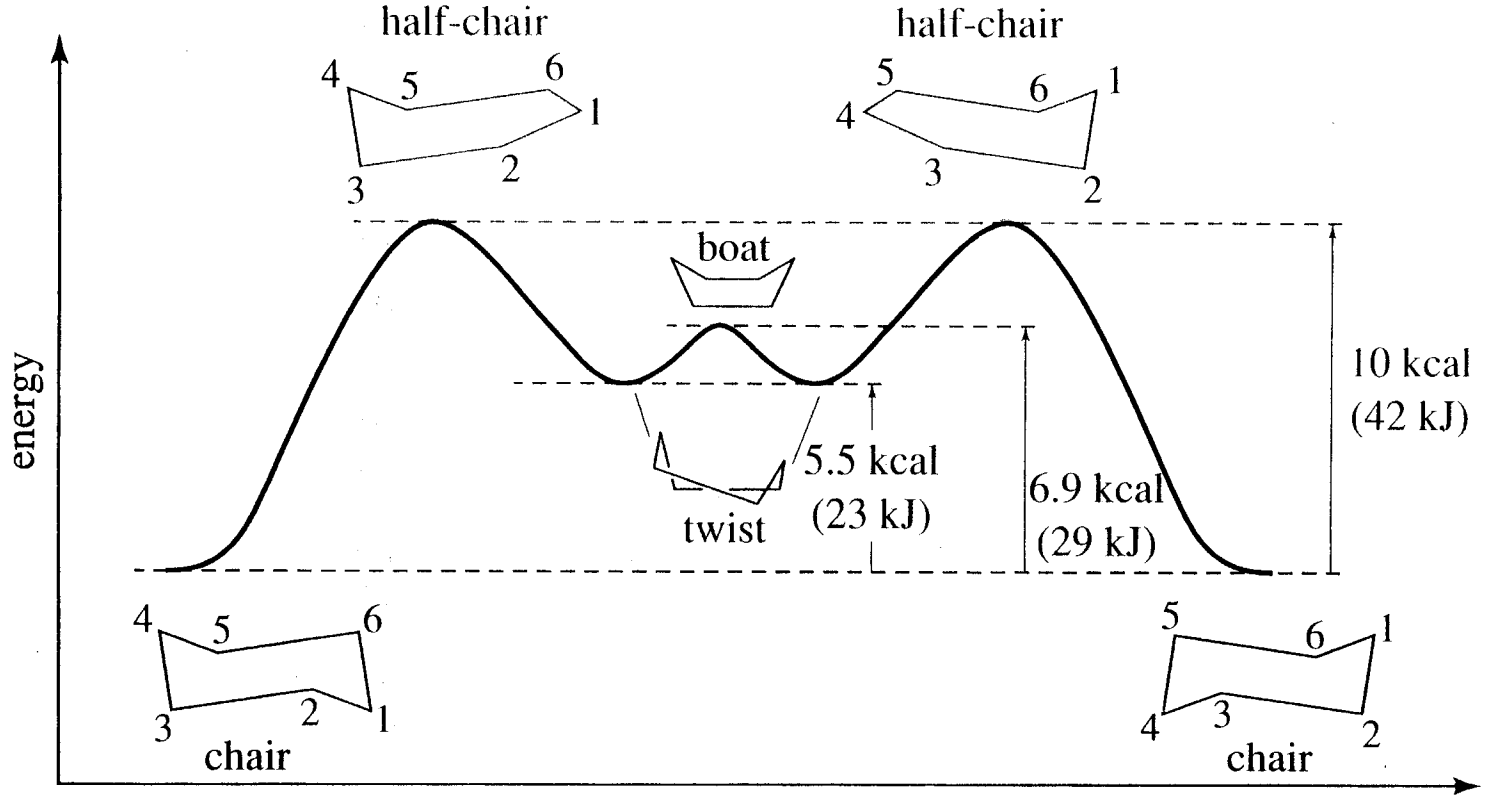
Newman projection

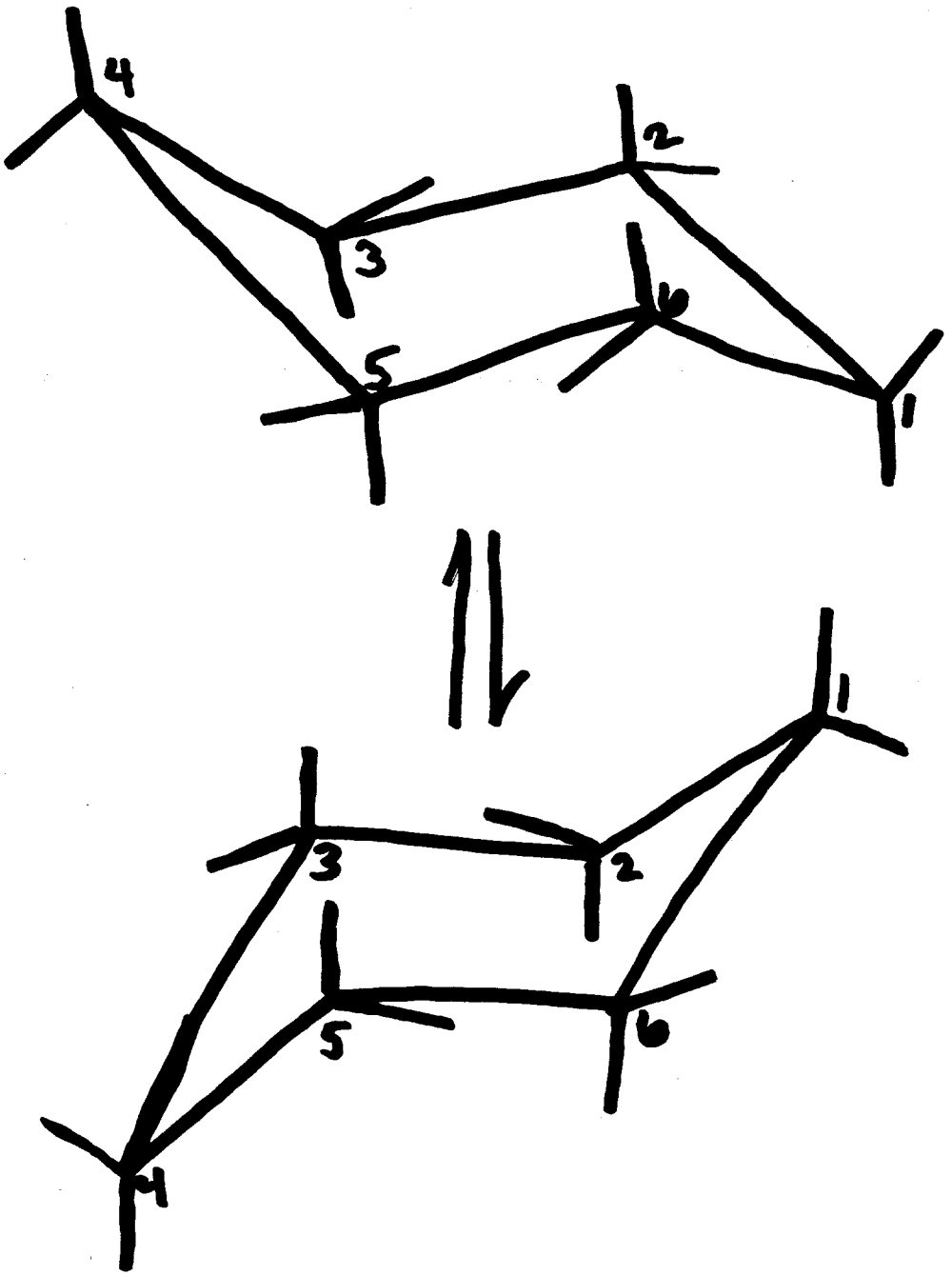


"twist" boat

T-21

Fig. 3-21 Energy of Cyclohexane Conformations

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