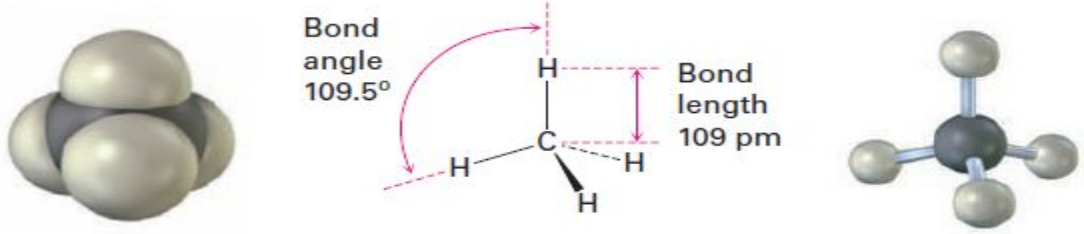
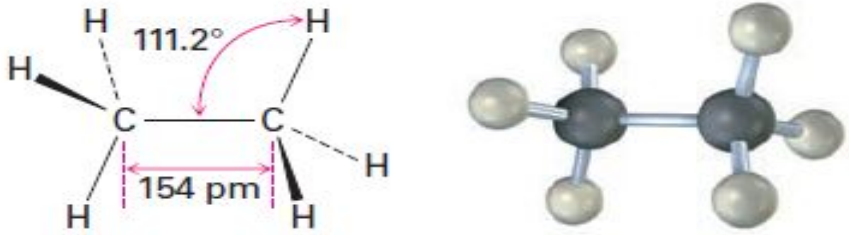
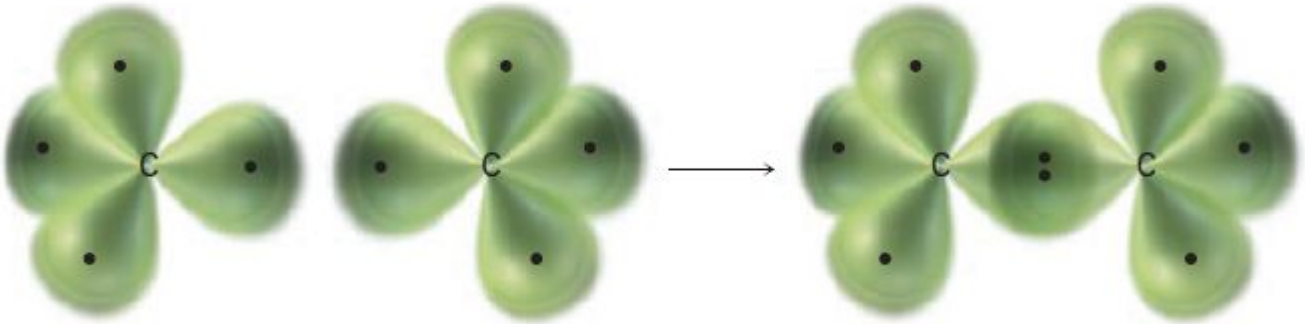
АЛКАНЫ
(строение и изомерия)





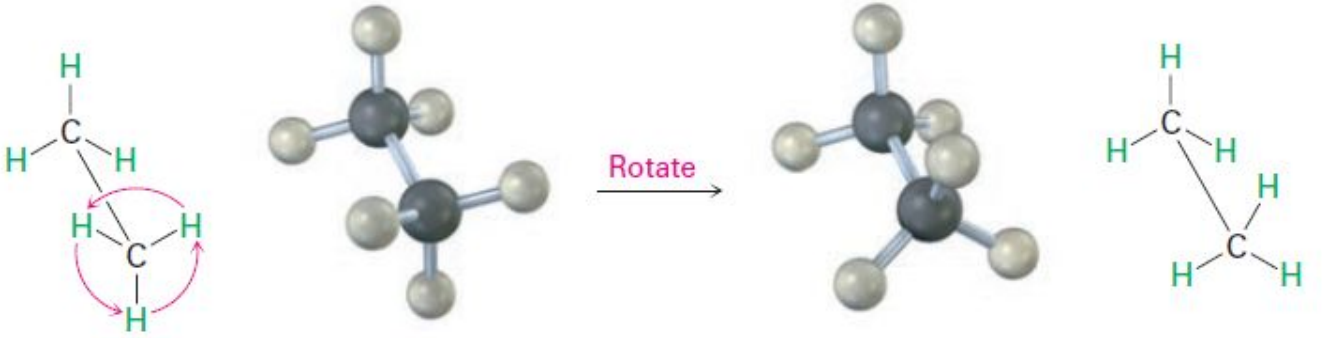
Ethane

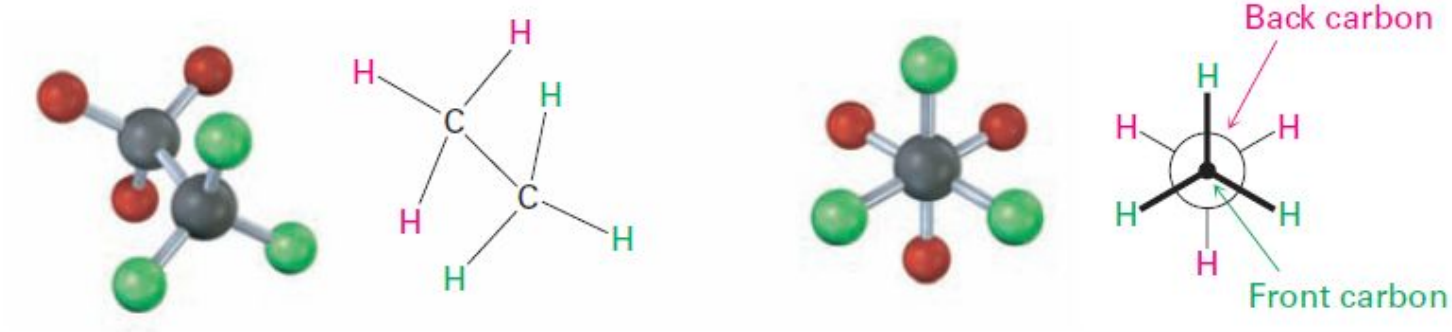


sp^3 carbon sp^3 carbon sp^3–sp^3 σ bond

Hexane

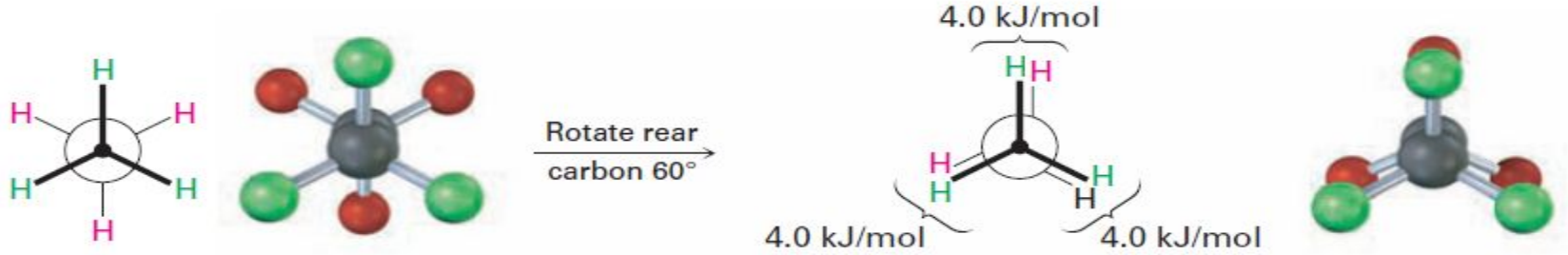
Конформации этана





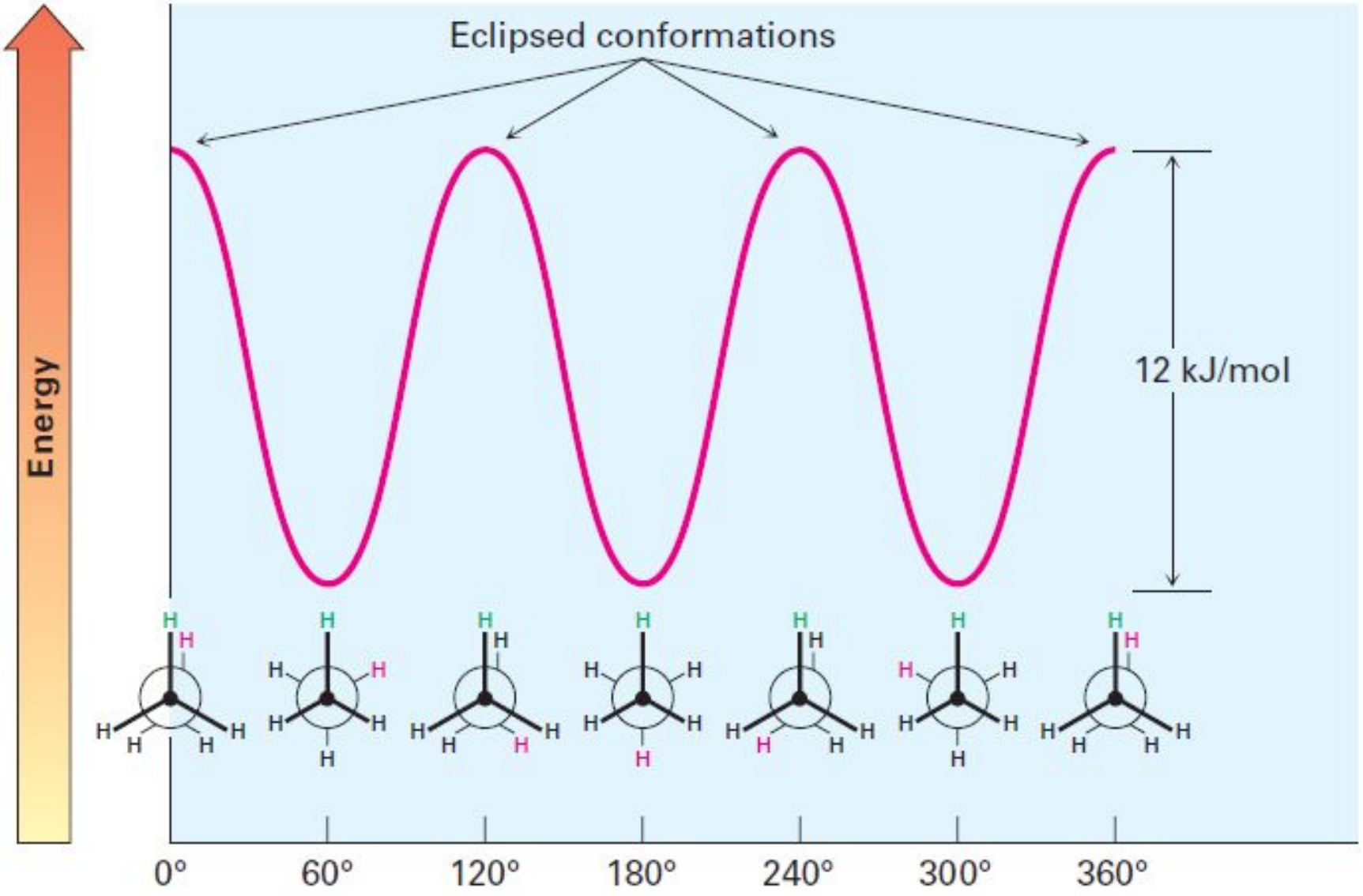
Sawhorse representation

Newman projection



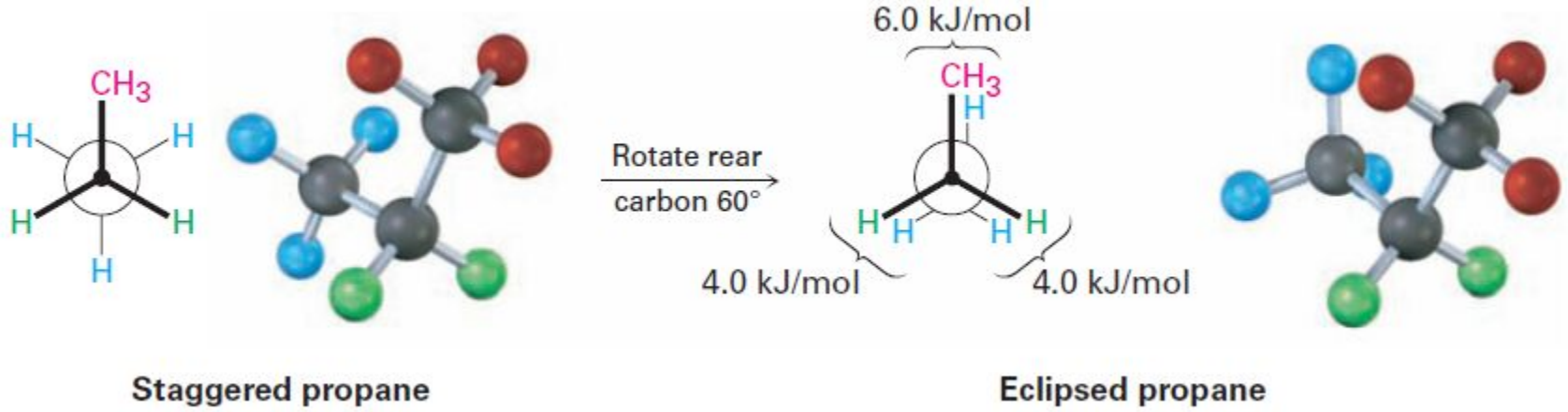
Ethane—staggered conformation

Ethane—eclipsed conformation

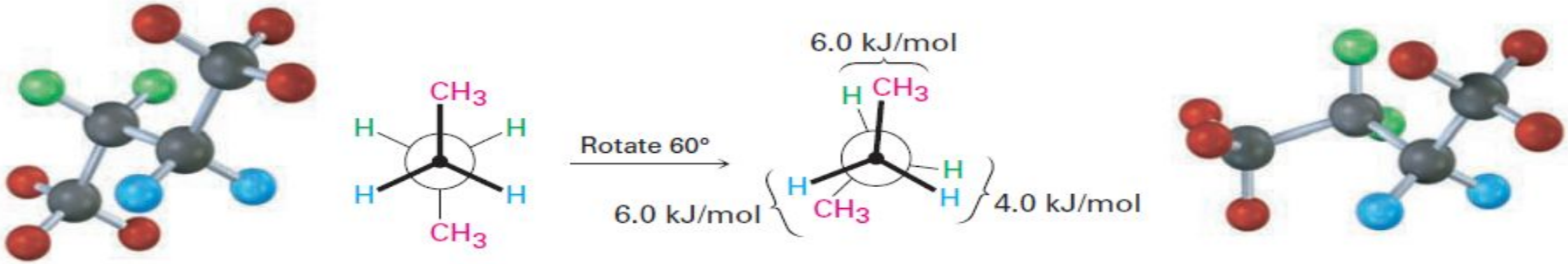

Eclipsed conformations
Energy
12 kJ/mol
H
0°
60°
120°
180°
240°
300°
360°

Конформации пропана и бутана

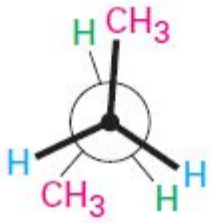
The eclipsed conformation of propane has three interactions—two ethane-type hydrogen–hydrogen interactions and one additional hydrogen–methyl interaction. Since each eclipsing H⟷H interaction is the same as that in ethane and thus has an energy "cost" of 4.0 kJ/mol, we can assign a value of $14 - (2 \times 4.0) = 6.0$ kJ/mol (1.4 kcal/mol) to the eclipsing H⟷CH_3 interaction



Staggered propane **Eclipsed propane**

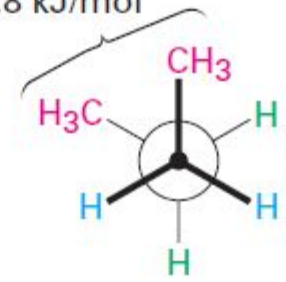


Butane—anti conformation (0 kJ/mol) **Butane—eclipsed conformation (16 kJ/mol)**



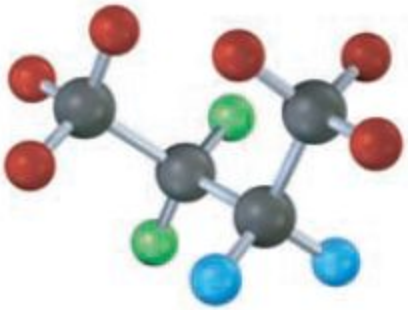
Rotate 60°

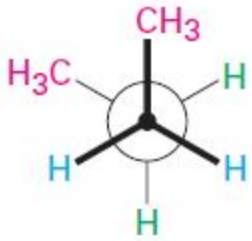
Steric strain
3.8 kJ/mol



Butane—eclipsed conformation (16 kJ/mol)

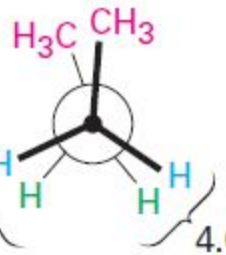
Butane—gauche conformation (3.8 kJ/mol)





Rotate 60°

11 kJ/mol



4.0 kJ/mol

4.0 kJ/mol

Butane—gauche conformation (3.8 kJ/mol)

Butane—eclipsed conformation (19 kJ/mol)

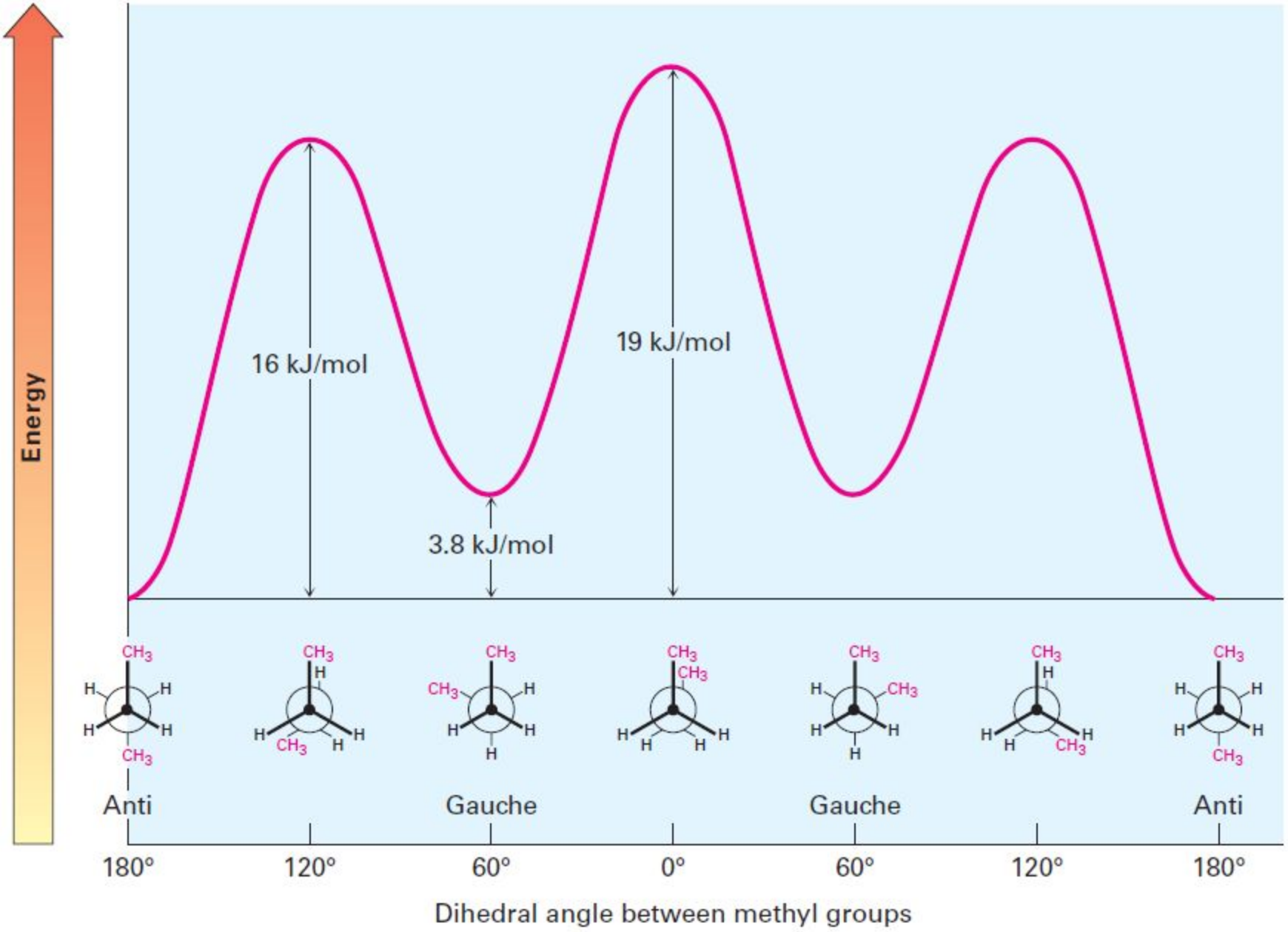

Energy
16 kJ/mol
19 kJ/mol
3.8 kJ/mol
Anti
Gauche
Gauche
Anti
180°
120°
60°
0°
60°
120°
180°
Dihedral angle between methyl groups

Table 3.5 Energy Costs for Interactions in Alkane Conformers

Interaction	Cause	Energy cost (kJ/mol)	Energy cost (kcal/mol)
H⟷H eclipsed	Torsional strain	4.0	1.0
H⟷CH_3 eclipsed	Mostly torsional strain	6.0	1.4
CH_3⟷CH_3 eclipsed	Torsional and steric strain	11	2.6
CH_3⟷CH_3 gauche	Steric strain	3.8	0.9

Sight along the C2—C3 bond of 2,3-dimethylbutane, and draw a Newman projection of the most stable conformation.

Draw a Newman projection along the C2—C3 bond of the following conformation of 2,3-dimethylbutane, and calculate a total strain energy:

Sight along the C2−C1 bond, 2-methylpropane (isobutane) and

(a) draw a Newman projection of the most stable conformation.

(b) draw a Newman projection of the least stable conformation.

(c) make a graph of energy versus angle of rotation around the C2−C1 bond.

(d) Since an H⟷H eclipsing interaction costs 4.0 kJ/mol and an H⟷CH_3 eclipsing interaction costs 6.0 kJ/mol, assign relative values to the maxima and minima in your graph.

Consider 2-methylbutane (isopentane). Sighting along the C2–C3 bond:

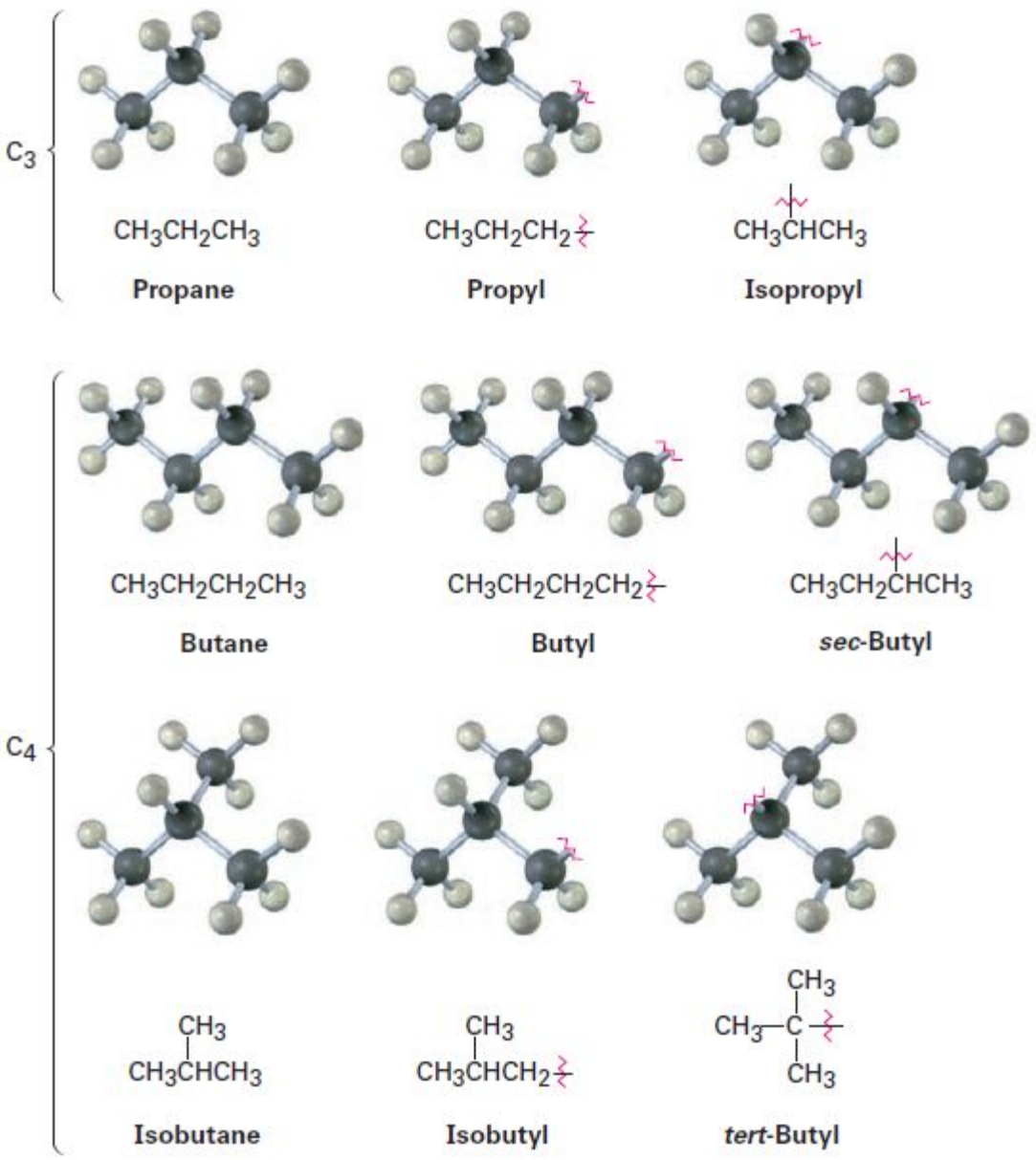
(a) Draw a Newman projection of the most stable conformation.

(b) Draw a Newman projection of the least stable conformation.

(c) If a $CH_3 \longleftrightarrow CH_3$ eclipsing interaction costs 11 kJ/mol (2.5 kcal/mol) and a $CH_3 \longleftrightarrow CH_3$ gauche interaction costs 3.8 kJ/mol (0.9 kcal/mol), make a quantitative plot of energy versus rotation about the C2–C3 bond.

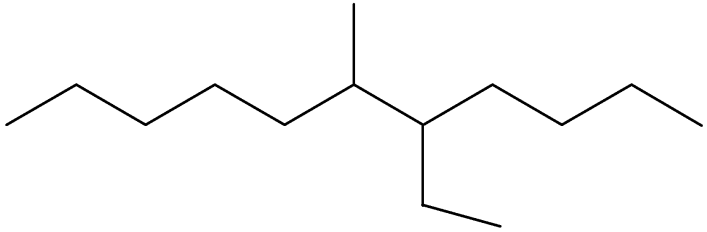
Construct a qualitative potential-energy diagram for rotation about the C−C bond of 1,2-dibromoethane. Which conformation would you expect to be most stable? Label the anti and gauche conformations of 1,2-dibromoethane.

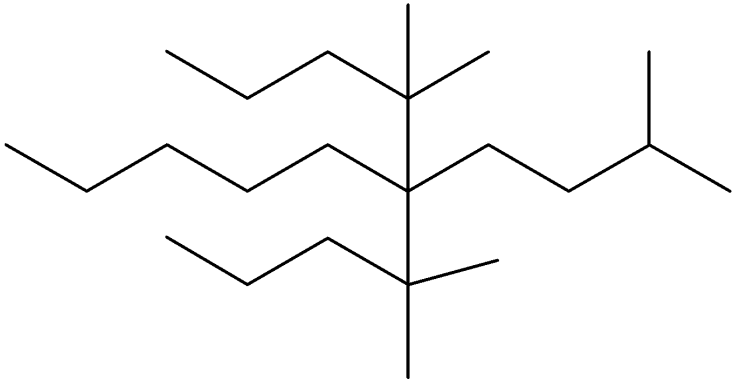
Алкильные группы

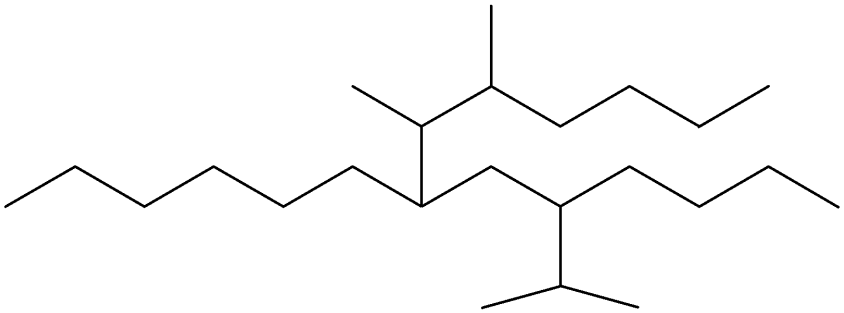


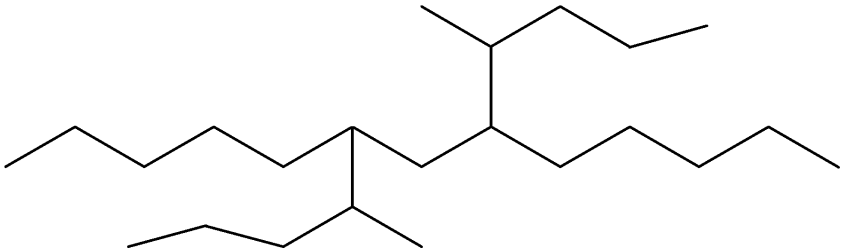
Locant — **Prefix** — **Parent** — **Suffix**

Where are the substituents and functional groups?	What are the substituents?	How many carbons?	What is the primary functional group?









Какой простейший алкан будет содержать энантиомер?