

# Chapter 2 – Alkanes

- Draw proper skeletal Lewis structures
  - Most organic molecules have some alkyl constituents.
- Conformational isomers
  - Dihedral angles
  - Rotatable bonds
- Constitutional isomers
- Physical properties

# Some properties of alkanes

- Fully saturated
  - $C_nH_{2n+2}$
  - No  $\pi$  bond or rings
- $sp^3$  hybridized carbon atoms, making 4  $\sigma$  bonds
- Not highly reactive, but
  - Cracking
  - Burning
  - Halogenation
  - Others
- Not acidic or basic
- Low boiling and melting points
- Nonpolar

# Alkane reactions (Ch 2.7)

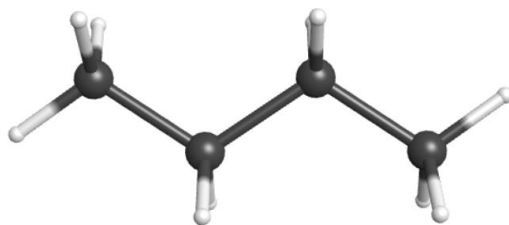
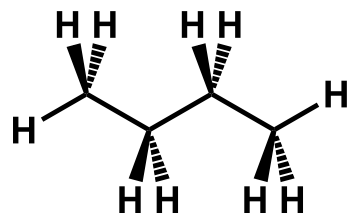
Thermal cracking

Combustion

Radical Halogenation

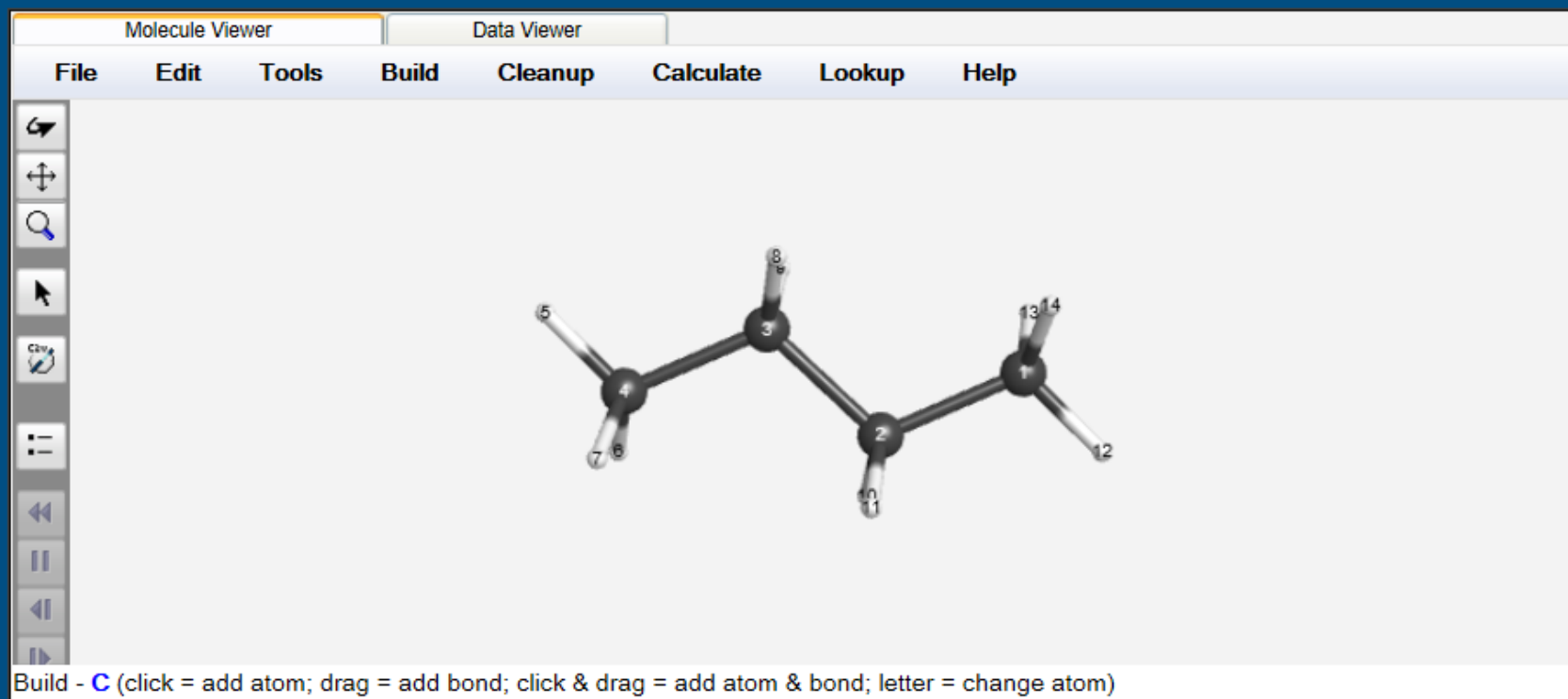
# Names and Lewis structure (Ch 2.4)

Simple unbranched alkanes



## WebMO Job Summary

114024: C<sub>4</sub>H<sub>10</sub> n-butane, Natural Bond Orbitals 6.0/NRT - Gaussian



Build - C (click = add atom; drag = add bond; click & drag = add atom & bond; letter = change atom)

Source:

[https://www.chem.wisc.edu/deptfiles/Corg/ch44WebMO/job\\_114024.html](https://www.chem.wisc.edu/deptfiles/Corg/ch44WebMO/job_114024.html)

June 30, 2021

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# Earth's atmosphere

Gas		% composition
Nitrogen	N <sub>2</sub>	78.084
Oxygen	O <sub>2</sub>	20.946
Argon	Ar	0.9340
Carbon dioxide	CO <sub>2</sub>	0.0397
Neon	Ne	0.001818
Helium	He	0.000524
Methane	CH <sub>4</sub>	0.000179
Water vapor	H <sub>2</sub> O	0.001%–5%

Methane is a greenhouse gas ~30 times more potent than CO<sub>2</sub>, and it has a lifetime of ~8.4 years in the atmosphere.

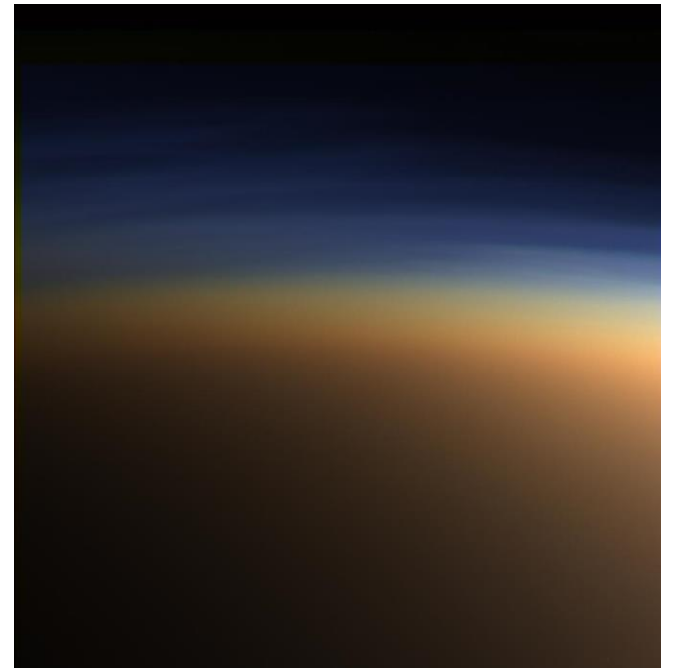
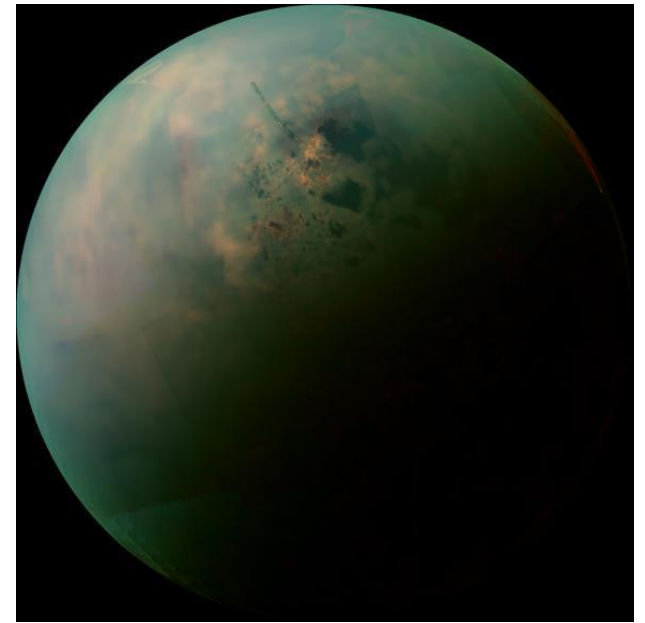
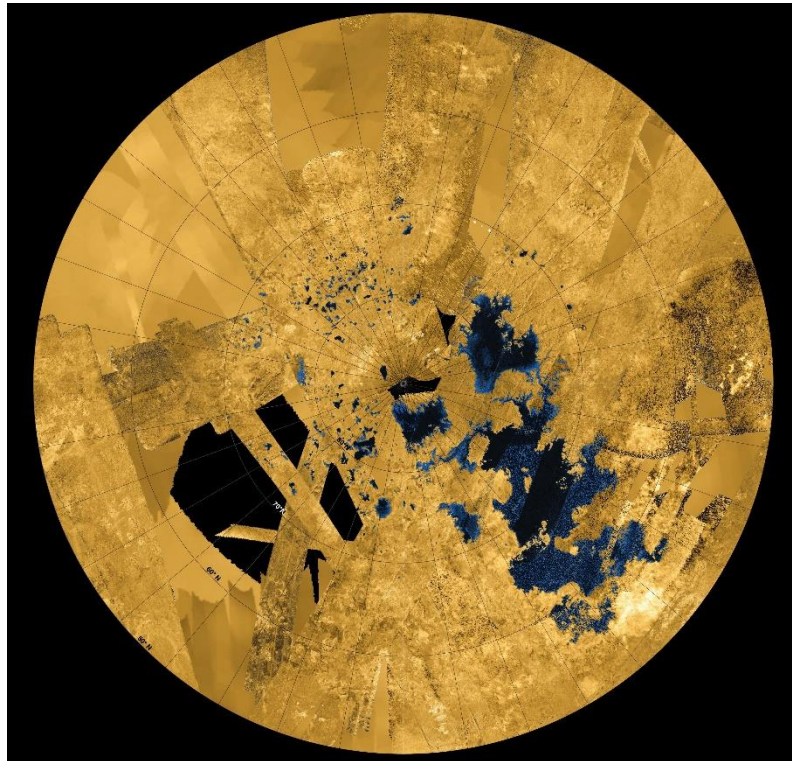
# Titan

The largest moon of Saturn

It has a dense atmosphere(1.45 atm) , which is unique for a moon

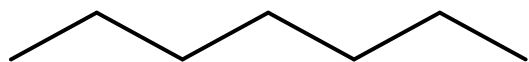
Its atmosphere at surface has 95%  $\text{N}_2$  and 4.9%  $\text{CH}_4$

Titan has ethane and methane lakes and seas!!!

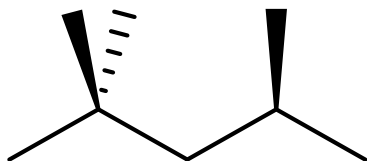


# Octane rating

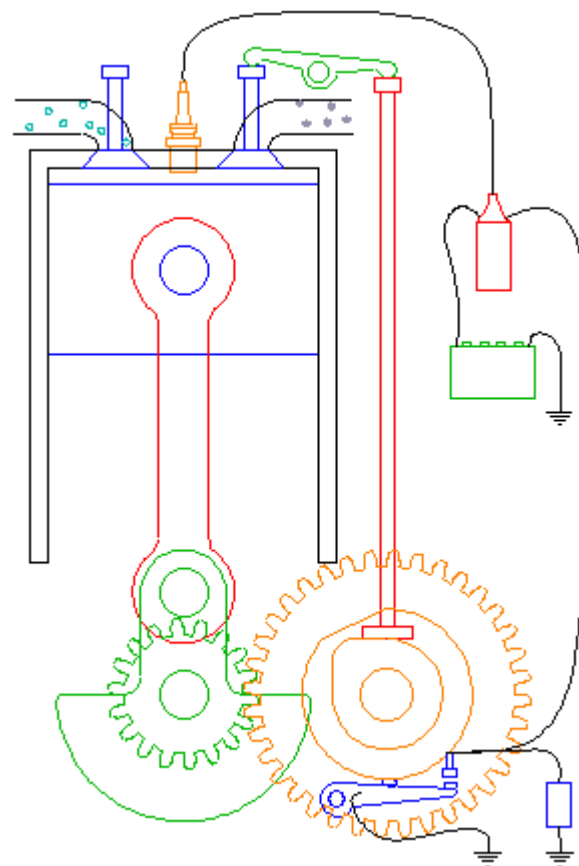
The higher the octane number, the more compression you can apply to the combustion chamber without the fuel detonating.



Heptane has an octane rating of 0



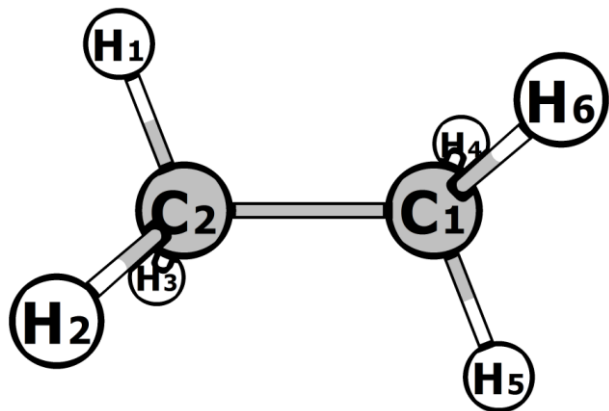
Isooctane has an octane rating of 100



<http://www.animatedengines.com/otto.html>

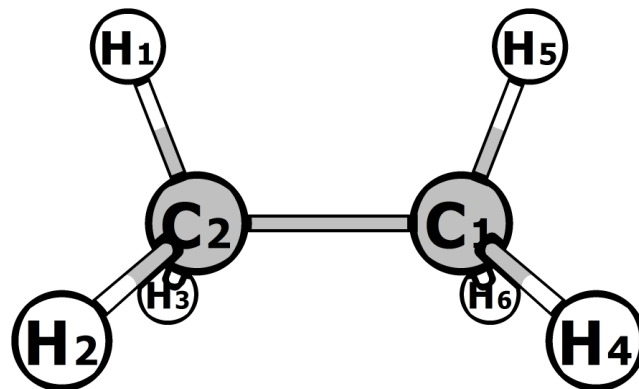


# Conformational isomerism (Ch 2.5)



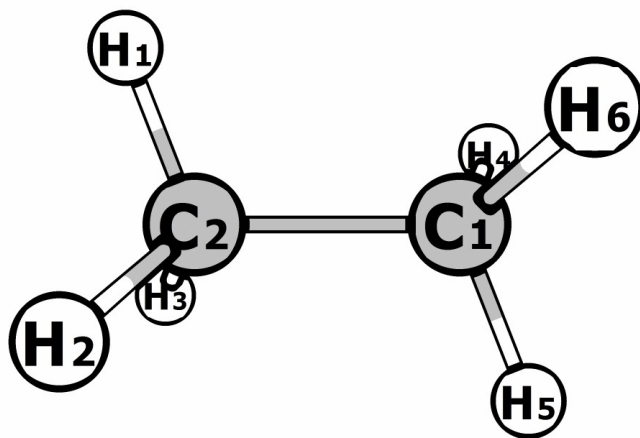
Staggered

H1-C2-C1-H5 dihedral angle =  $180^\circ$



Eclipsed

H1-C2-C1-H5 dihedral angle =  $0^\circ$



# Newman projection – *Staggered* Ethane



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Preview

# Newman projection – *Eclipsed* Ethane



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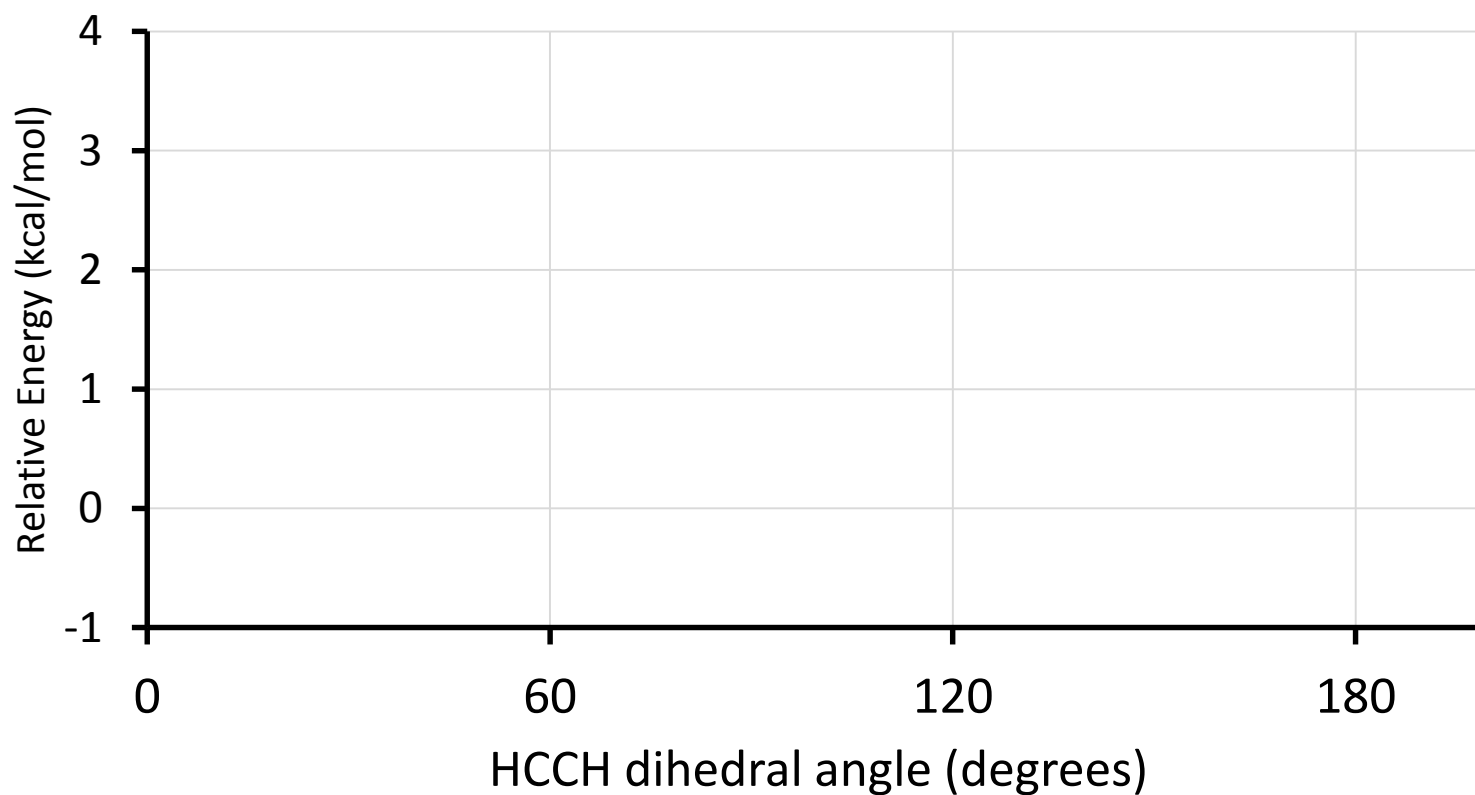
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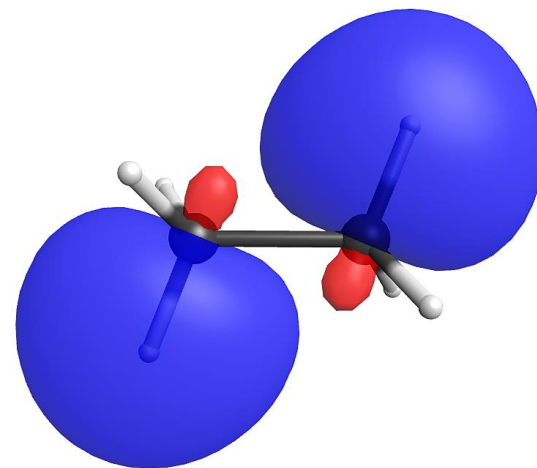
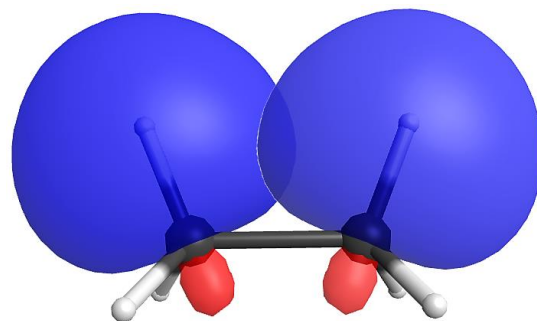
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Preview

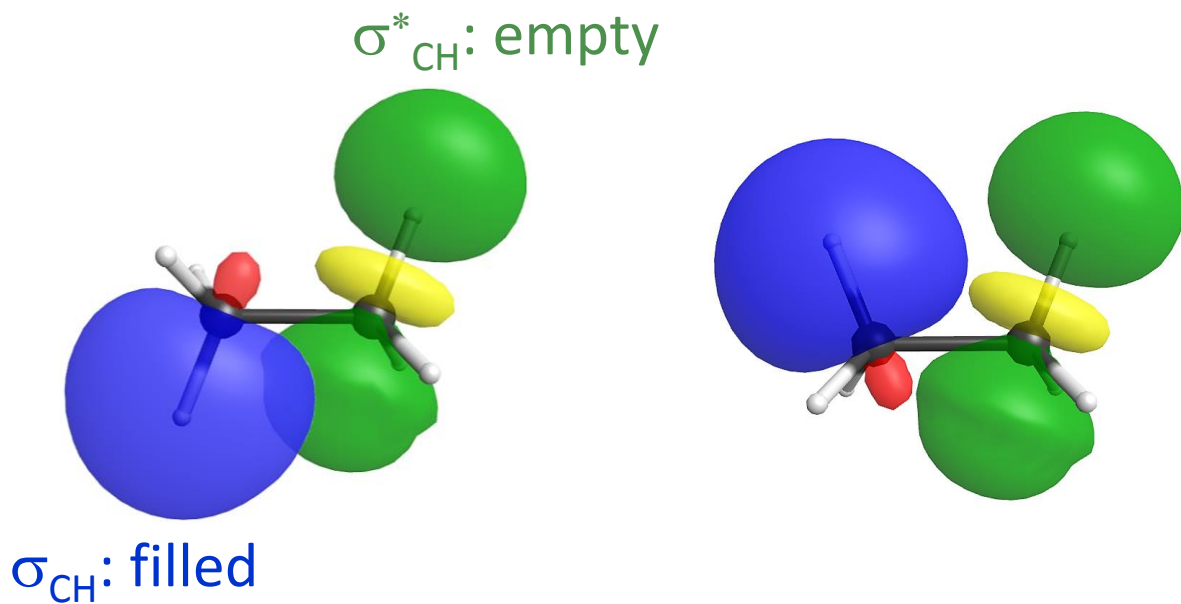
# Ethane conformations

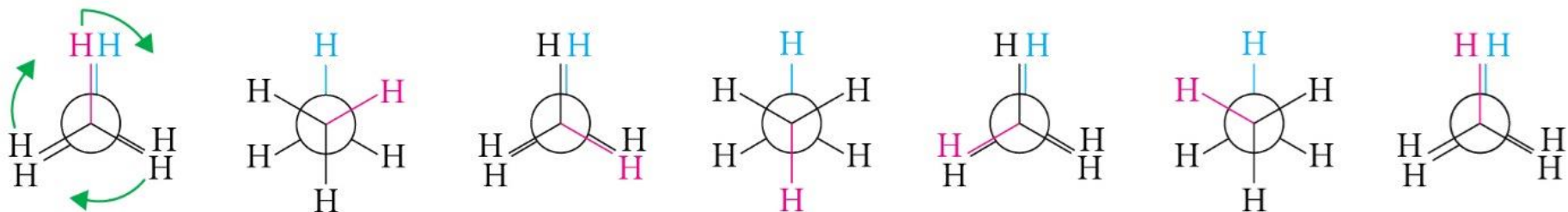
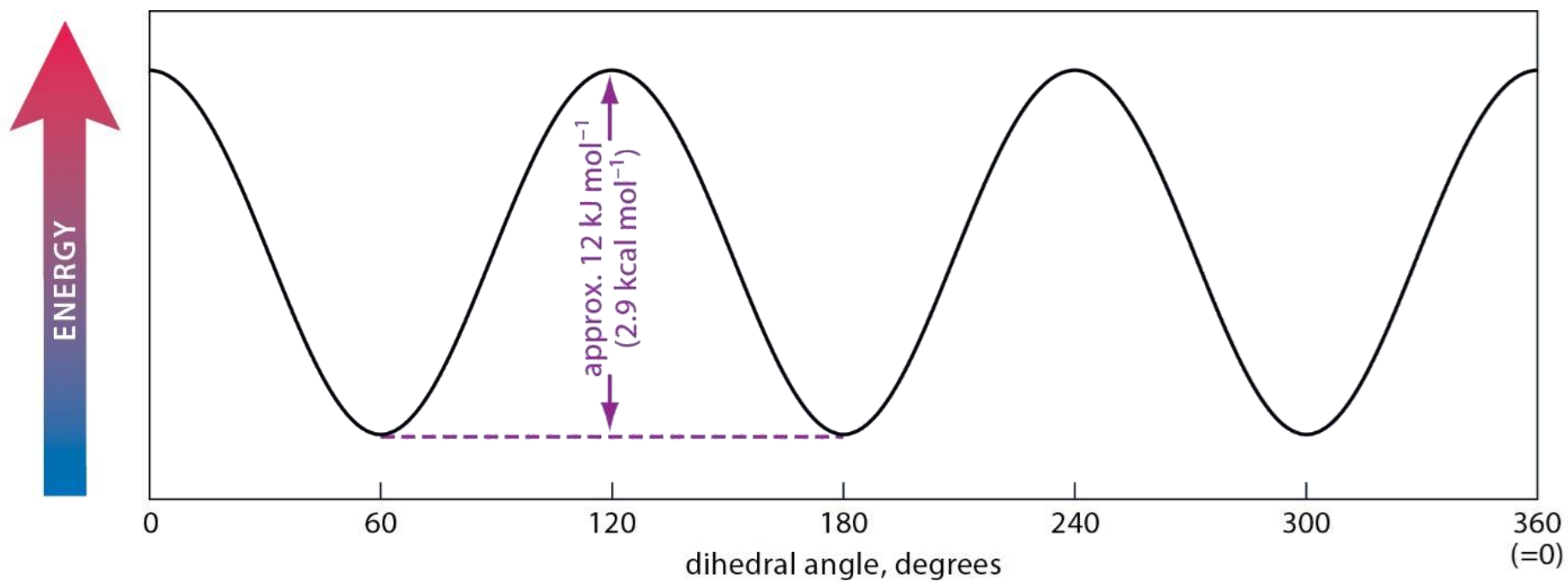


# $e^- - e^-$ repulsion



# Hyperconjugation

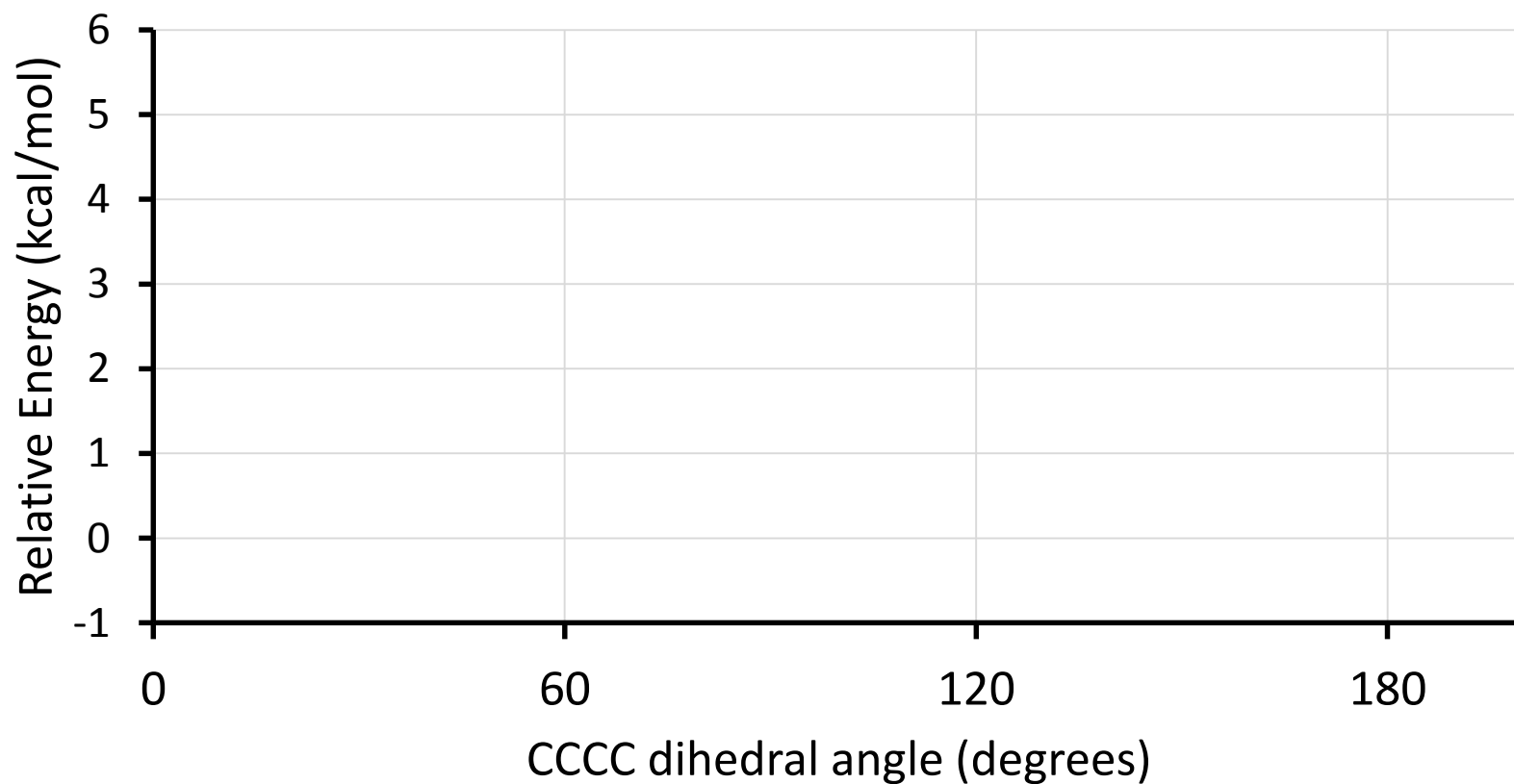




# Butane conformations



# Butane conformations



# Constitutional Isomers ( $\text{C}_6\text{H}_{14}$ )

Alkane	Formula	Boiling point [°C]	Melting point [°C]	Density [g·cm <sup>-3</sup> ] (at 20 °C)
Methane	CH <sub>4</sub>	-162	-182	gas
Ethane	C <sub>2</sub> H <sub>6</sub>	-89	-183	gas
Propane	C <sub>3</sub> H <sub>8</sub>	-42	-188	gas
Butane	C <sub>4</sub> H <sub>10</sub>	0	-138	gas
Pentane	C <sub>5</sub> H <sub>12</sub>	36	-130	0.626 (liquid)
Hexane	C <sub>6</sub> H <sub>14</sub>	69	-95	0.659 (liquid)
Heptane	C <sub>7</sub> H <sub>16</sub>	98	-91	0.684 (liquid)
Octane	C <sub>8</sub> H <sub>18</sub>	126	-57	0.703 (liquid)
Nonane	C <sub>9</sub> H <sub>20</sub>	151	-54	0.718 (liquid)
Decane	C <sub>10</sub> H <sub>22</sub>	174	-30	0.730 (liquid)
Undecane	C <sub>11</sub> H <sub>24</sub>	196	-26	0.740 (liquid)
Dodecane	C <sub>12</sub> H <sub>26</sub>	216	-10	0.749 (liquid)
Hexadecane	C <sub>16</sub> H <sub>34</sub>	287	18	0.773 (liquid)
Icosane	C <sub>20</sub> H <sub>42</sub>	343	37	solid
Triacontane	C <sub>30</sub> H <sub>62</sub>	450	66	solid
Tetracontane	C <sub>40</sub> H <sub>82</sub>	525	82	solid
Pentacontane	C <sub>50</sub> H <sub>102</sub>	575	91	solid
Hexacontane	C <sub>60</sub> H <sub>122</sub>	625	100	solid