13.6 Alkadienes and Polyunsaturated Hydrocarbons
A hydrocarbon whose molecules contain two double bonds is called an alkadiene (alkatriene for three double bonds);

A hydrocarbon with two triple bonds is called an alkadiyne;

A hydrocarbon with a double and triple bond is called an alkenyne.

\[
\begin{align*}
\text{HC≡C−CH}_2−\text{C≡CH} & \quad \text{An alkadiyne} \\
\text{HC≡C−CH}_2−\text{CH}=\text{CH}_2 & \quad \text{An alkenyne}
\end{align*}
\]
- **Cumulated dienes** — The molecules have cumulated double bonds
- **Isolated dienes** — one or more saturated carbon atoms intervene between the double bonds of an alkadiene.
- **Conjugated dienes** — the double and single bonds alternate along the chain

\[
\begin{align*}
\text{C= C= C} & \quad \text{A cumulated diene} \\
\text{C= C}\quad \text{C= C} & \quad \text{A conjugated diene} \\
\text{C= C}\quad (\text{CH}_2)_n\quad \text{C= C} & \quad \text{An isolated diene (n \neq 0)}
\end{align*}
\]
Chapter 13

13.7 1,3-Butadiene: Electron Delocalization
13.7A Bond Lengths of 1,3-Butadiene

All of the 1,3-butadiene are $sp^2$ hybridized and as a result, the central bond of butadiene results from overlapping $sp^2$ orbitals.

Bond lengths

\[ \text{C} = \text{C} \quad 154 \text{ pm} \]
\[ \text{C} - \text{C} \quad 134 \text{ pm} \]

\[ \text{CH}_2\text{=CH} \quad 133.7 \text{ pm} \]
\[ \text{CH=CH}_2 \quad 146 \text{ pm} \]
13.7B Conformations of 1,3-Butadiene

- s-cis conformation
- s-trans conformation

s-cis and s-trans conformations can be interconverted through rotation about the single bond.

The s-trans conformation is the predominant one at room temperature.
13.7C Molecular Orbitals of 1,3-Butadiene

- **HOMO** — (highest occupied molecular orbital)
- **LUMO** — (lowest unoccupied molecular orbital)
13.8 The Stability of Conjugated Dienes
Conjugated alkadienes are thermodynamically more stable than isomeric isolated alkadienes.

**Heats of hydrogenation**

\[
\begin{align*}
\text{CH}_3\text{CH}_2\text{CH}=&\text{CH}_2 & \text{CH}_2=&\text{CH}—\text{CH}=&\text{CH}_2 \\
\Delta H^\circ & 127 \text{ kJ / mol} & 239 \text{ kJ / mol} \\
\Delta H^\circ / \text{C}=&\text{C} & 127 \text{ kJ / mol} & 119.5 \text{ kJ / mol}
\end{align*}
\]