Writing Organic Structures

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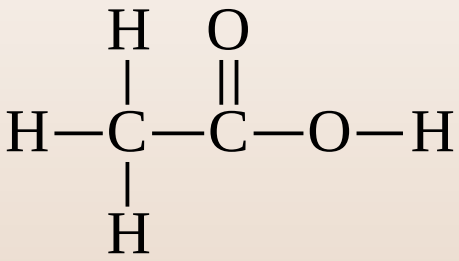
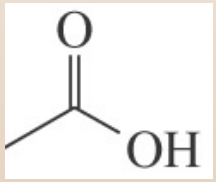
Chemical Formulas

- Full structural formula (no lone pairs shown)



- Line-angle formula

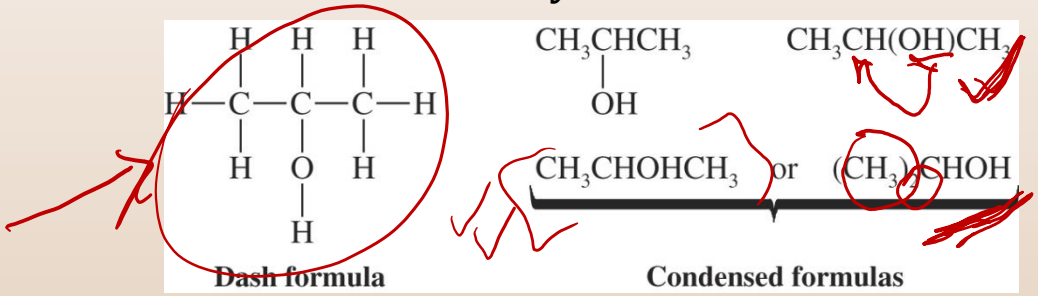


- Condensed structural formula
- Molecular formula
- Empirical formula

- CH_3COOH
- $C_2H_4O_2$
- CH_2O

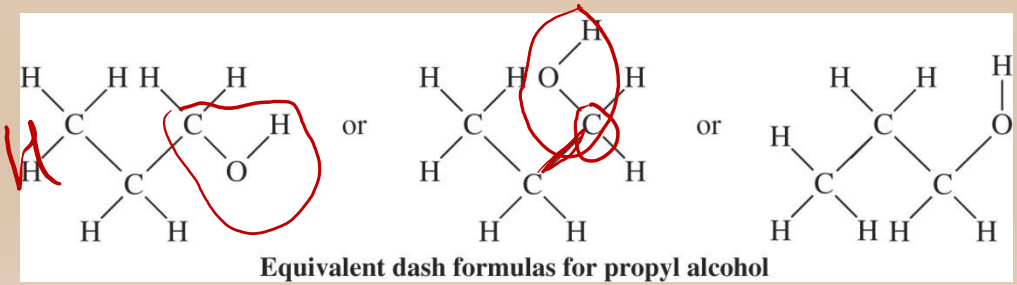
Condensed Structural Formulas

- In these representations, generally all lines are omitted
- In partially condensed structures all hydrogens attached to an atom are simply written after it but in some, bonds are explicitly shown
- In fully condensed structure all bonds are omitted and atoms attached to carbon are written immediately after it

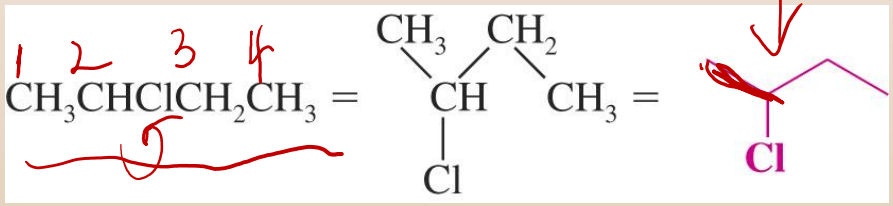


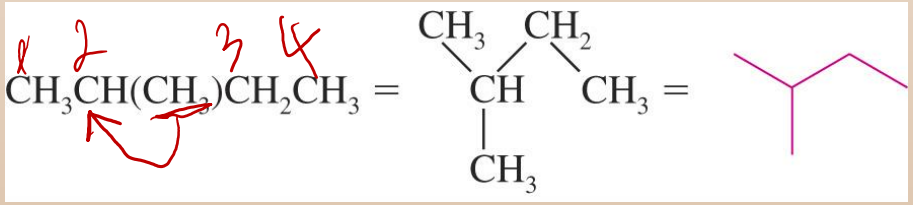
Expanded (Dash) formulas

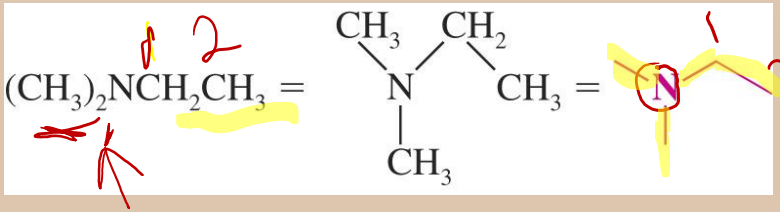
- Each line represents a pair of electrons
- This type of representation is meant to emphasize connectivity and does not represent the 3-dimensional nature of the molecule
- There is free rotation around single bonds so the structures below are all equivalent

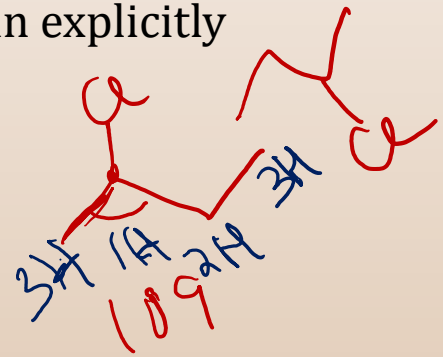


- **Line Formulas**
  - A further simplification of drawing organic molecules is to completely omit all carbons and hydrogens and only show heteroatoms (*e.g.* O, Cl, N) explicitly
  - Each intersection or end of line in a zig-zag represents a carbon with the appropriate amount of hydrogens
    - Heteroatoms with attached hydrogens must be drawn in explicitly

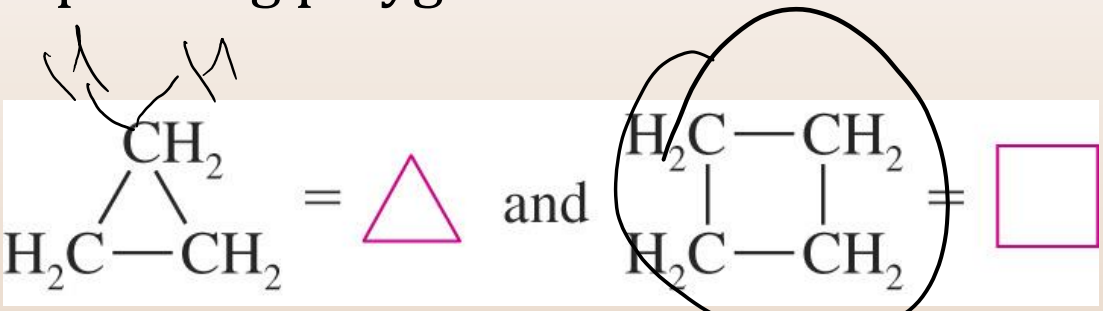


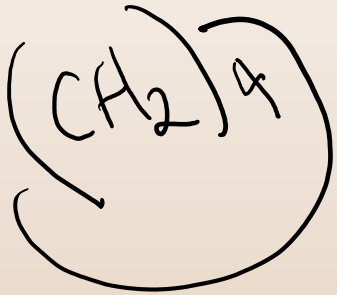




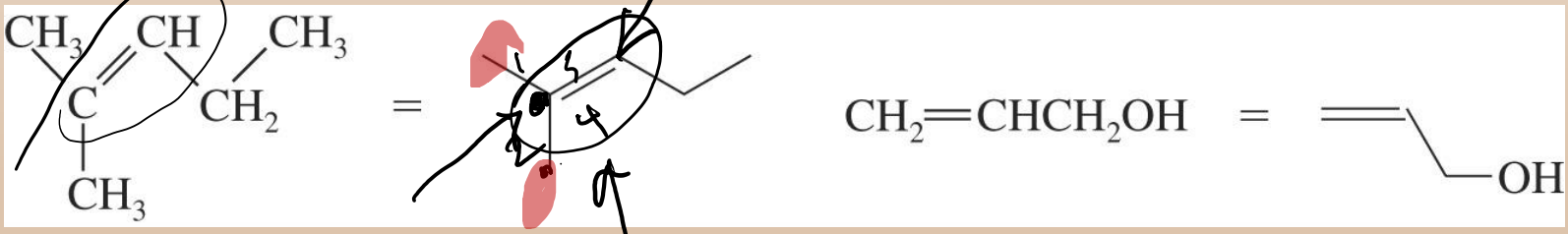


- Cyclic compounds are condensed using a drawing of the corresponding polygon



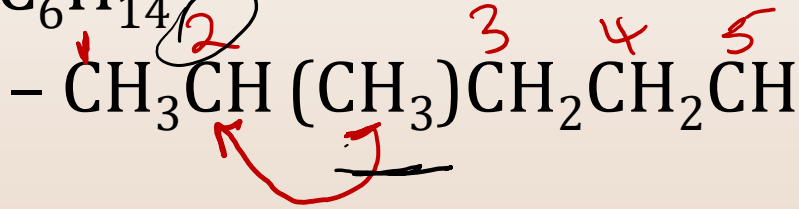


- Multiple bonds are indicated by using the appropriate number of lines connecting the atoms

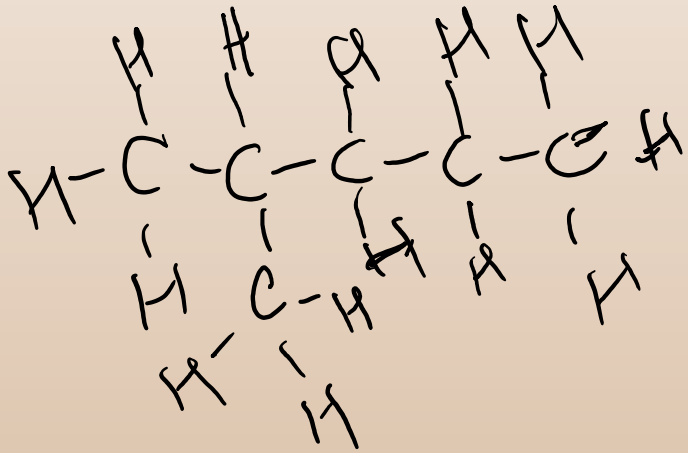


An Example

- Molecular Formula – C_6H_{14}
- Condensed Structure – $CH_3CH(CH_3)CH_2CH_2CH_3$

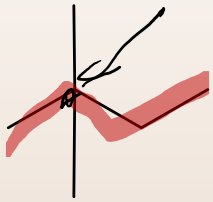


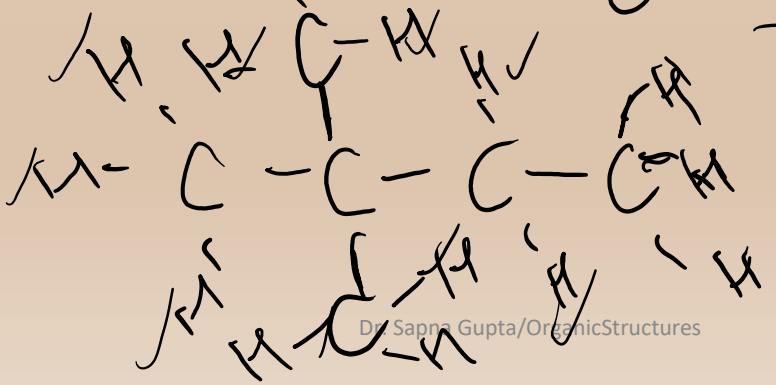
- Expanded structure –



- Line structure –

Another Example

- Line structure – 
- Molecular Formula – C_6H_{14}
- Condensed Structure – $CH_3C(CH_3)_2CH_2CH_3$ $(CH_3)_3CCH_2CH_3$
- Expanded structure – $CH_3CH_3CH_3CH_2CH_3$



Key Words/Concepts

Writing Organic Compounds

- Molecular formula
- Structural formula
- Line structure
- Expanded structure