This tutorial is made by Karina Koval
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SMILES Tutorial

Denote any inorganic atom with brackets. Organic elements may be written using capital letters without brackets. It is unnecessary to include the Hydrogens attached to the organic elements unless the atom is charged.

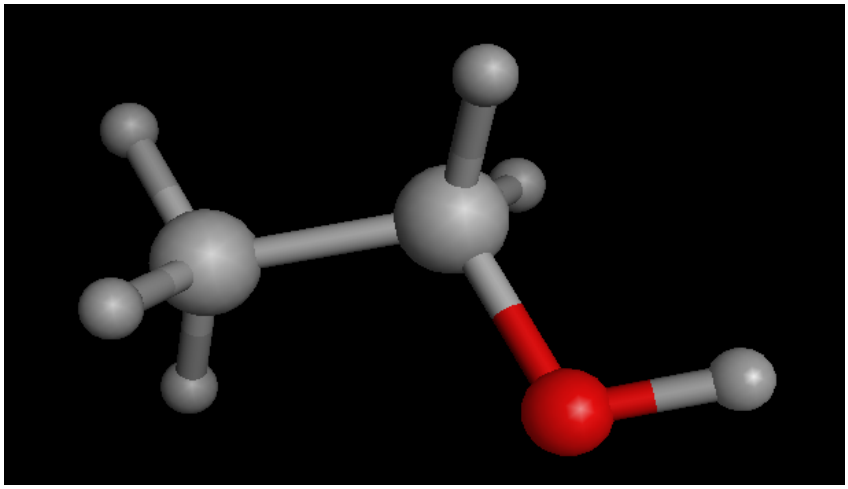
Examples: [Ag] –Silver.

In order to denote charged atoms, the atom must be followed by the symbol for Hydrogen (H) if any excess hydrogens are bonded to the central atom, and the charge of the atom. Charged compounds must be put in brackets.

Examples: [OH-] denotes hydroxide, [OH3+] denotes Hydronium

Single bonds can be denoted by dashes (-), however, they are not necessary. You can denote single bonds by adjacency of atoms.

Example:



Ethanol – CCO

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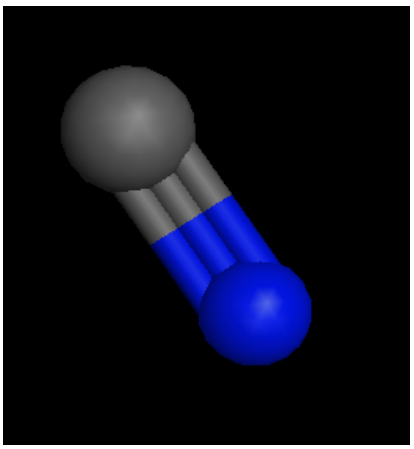
Double bonds are denoted by the equal sign (=), and triple bonds are denoted by the pound sign (#).

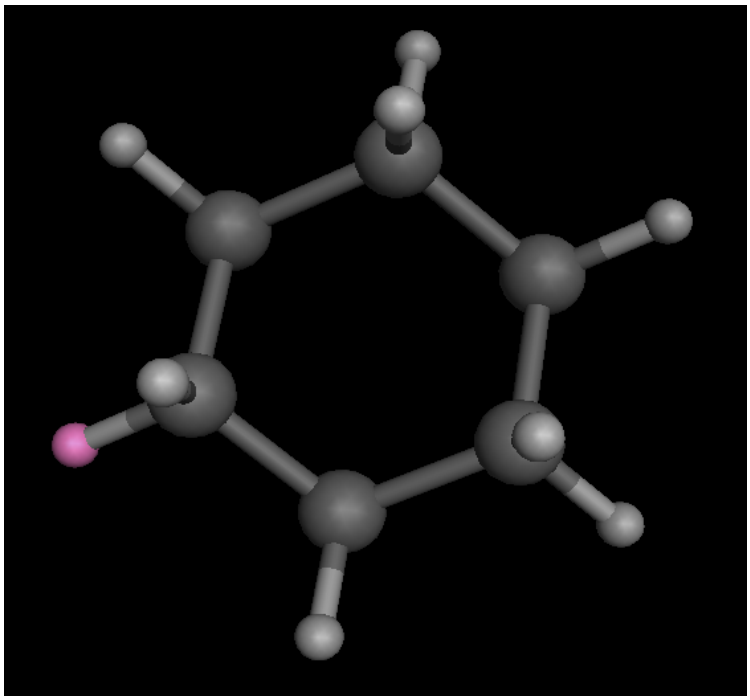
Example:



Cyanide – [C-]#N

Rings are denoted by numbering atoms which are connected to each other.

Examples:



Cyclohexane:

C1CCCCC1

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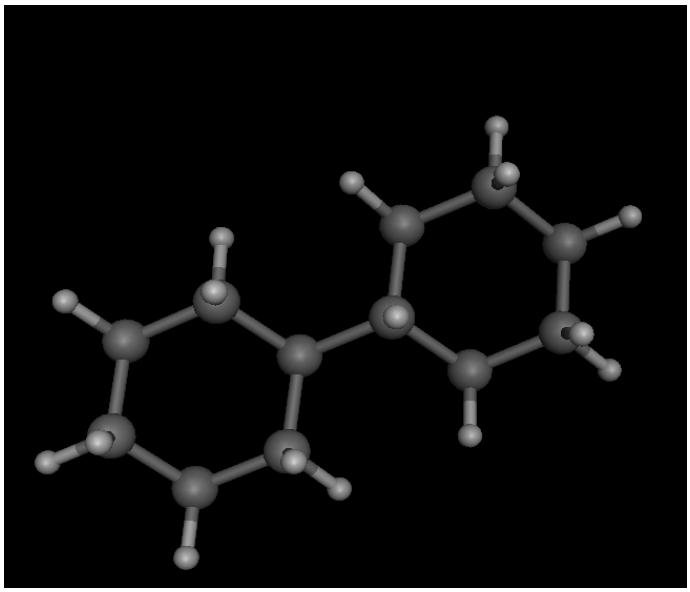
Branching in molecules is denoted by parenthesis.

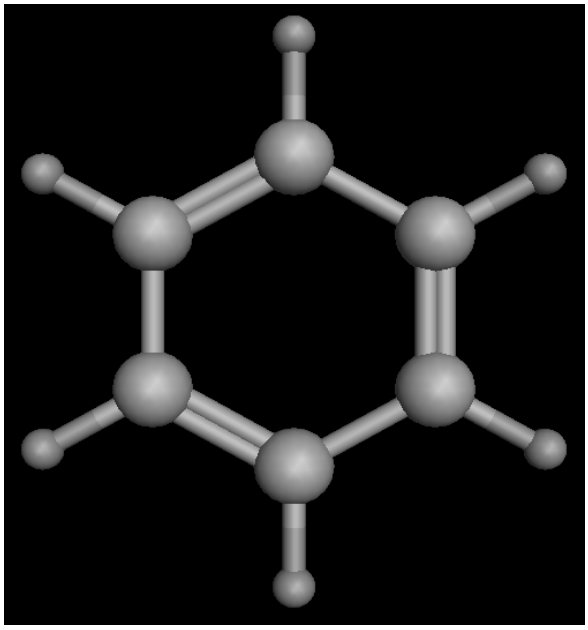
Example:



Cyclohexylcyclohexane - C1CCC(CC1)C2CCCCC2

Aromatic compounds (Oxygen, Carbon, Nitrogen and Sulfur) are written in lowercase.

Example:



Benzene – c1ccccc1

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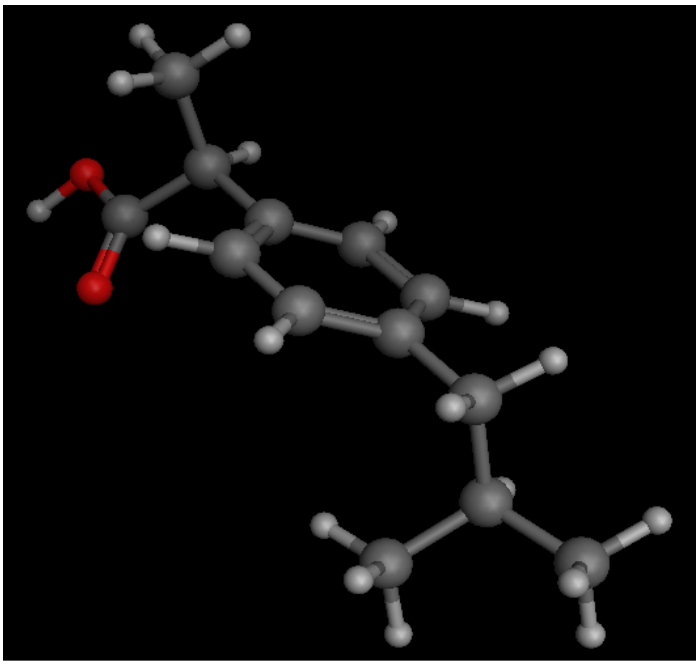
Chirality is denoted by @ (anticlockwise) and @@ (clockwise). E and Z isomerism around a double bond is denoted by slashes. Two slashes of one type denote trans configuration, and two opposite facing slashes denote cis configuration. (\\, // both denote trans, /\,\/, both denote cis)

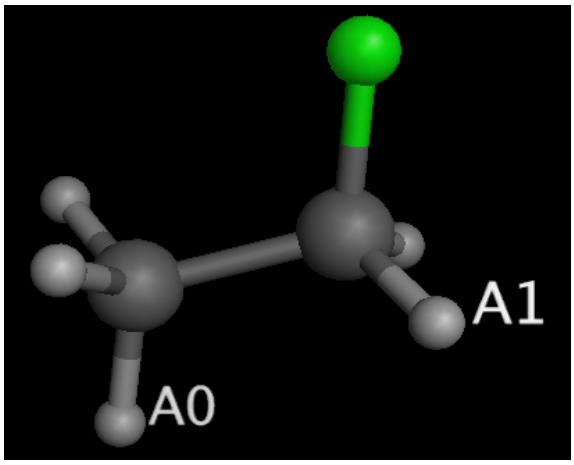
Example:



S-ibuprofen - OC(=O)[C@@H](C)c1ccc(cc1)CC(C)C

To denote the head and tail of a polymer, use [(*)] after the atom which is connected to other repeating units. The asterisk acts just a hydrogen atom.

Examples:



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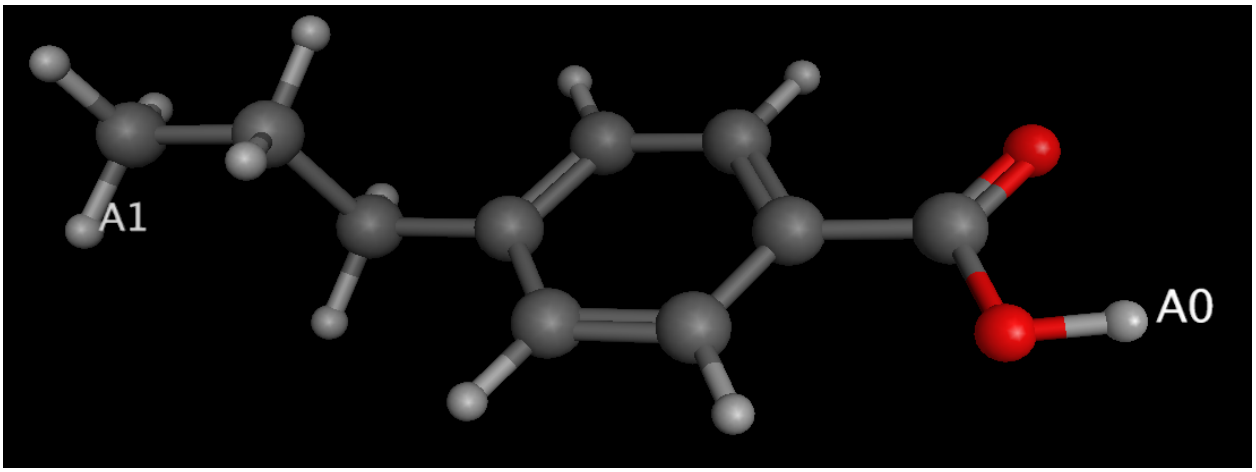
Polyvinylfluoride – C([*])[C@@H]([*])F



O[(*)]C(=O)c1ccc(cc1)CCC[(*)]

Note: Polymer Design Platform can't currently handle ladder polymers or charged units.

For a formal tutorial of SMILES, you can visit the Daylight SMILES Tutorial - http://www.daylight.com/dayhtml/doc/theory/theory.smiles.html