



Acceleration

STEM Sims

Lesson 7: 100 Octane Rating

Iso-octane is the most important ingredient in gasoline. Although gasoline contains around 18 different chemicals, iso-octane is the one that gives gasoline an octane rating of 100. The higher the octane rating, the more energy produced when the gasoline combusts. A zero (0) rating is given to gasoline containing only *n*-heptane, so you would not want to try to operate a vehicle using only this chemical. In this investigation, you'll discover the wonders of organic chemicals and learn a great way to impress your friends and family when you draw the structure of some complex chemicals.

Doing the Science

1. This investigation is a paper and pencil exercise. You do *not* need access to the simulation to complete this activity.
2. The “real” name of iso-octane is 2,2,4-trimethylpentane. This is a hydrocarbon consisting only of carbon and hydrogen. Now the real fun begins. If you want to draw the structure of the compound, always start at the rear of the name. The main group is listed last in the name. In this case, pentane is the main group. To draw pentane, you'll need Table 1.

Table 1

Number of Carbon Atoms in Main Group	Prefix
1	Meth
2	Eth
3	Prop
4	But
5	Pent
6	Hex
7	Hept
8	Oct
9	Non
10	Dec

3. Target molecule = 2,2,4-trimethylpentane
Since pentane is the target, use the above table and see that pentane has 5 carbon atoms in the main group. The -ane ending is because all of the carbon atoms are singly bonded to each other. Write 5 “C’s” in a row, connecting each with a “—” to represent a chemical bond between each carbon atom.
4. Number each “C” (carbon atom) 1 - 5. Since each carbon atom must make 4 bonds, place three “—” around carbons 1 and 5, and two “—” above and below carbons 2 - 4.

5. A side group is an atom or group of atoms other than hydrogen connected to the main group. Iso-octane (2,2,4-trimethylpentane) has side groups. To show a side group, the ending on the side group is changed to “-yl.” Side groups are listed before the main group. In this case, the side group is methyl. Again, using Table 1, “meth” has 1 carbon atom. But there’s a prefix “tri” in front of the methyl side group. To figure out what the “tri” means, you’ll need Table 2 below.

Table 2.

Number of Side Groups	Prefix
1	Mono
2	Di
3	Tri
4	Tetra
5	Penta
6	Hexa
7	Hepta
8	Octa
9	Nona
10	Deca

6. Did you figure out how many “methyl” groups in this molecule? If you answered three, you are correct. Trimethyl means there are three one-carbon side groups attached to the main group. Now the question is where to place the three side groups? Remember how you numbered the carbon atoms in the main group, that’s where the side groups attach. Attach one “C” to the top of the #2 carbon in the main group, another “C” to the bottom of that same carbon in the main group, and the last “C” to the #4 carbon in the main group.
7. Again, since all “C’s” must have four total chemical bonds, place three “—” around each side group “C”. You should place a total of nine “—”.
8. Lastly, write an “H” to represent a hydrogen atom at the end of any “—” that is *not* attached to another “C”. And behold, you have created the structure of iso-octane (2,2,4-trimethylpentane).

Do You Understand?

1. Write the chemical formula of 2,2,4-trimethylpentane. Explain why the molecule is called “octane”.
2. Draw the structure of the following molecules:
 - a. 2,4-dimethylhexane
 - b. 3,3,4,4-tetramethylnonane