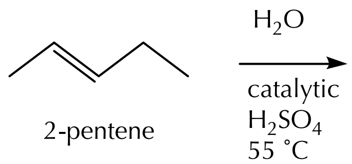
Your prior knowledge about organic molecules is also useful, such as, the well-behaved nature of the main group organic elements: You can bet that the carbons will have 4 bonds, the oxygen will have 2 bonds, and the hydrogens will each have 1 bond. Another useful fact is that the $C_5H_{12}O$ molecular formula has no units of unsaturation, and just like 2-pentanol and 3-pentanol, the unknown compound C can have no rings or multiple bonds in its structure.

A surprising but inescapable hypothesis is that the connectivity of the carbon atoms has changed. The 2-pentanol and 3-pentanol connectivities are already given, and the single other $C_5H_{12}O$ alcohol with all five carbons in a row is 1-pentanol. The 1-pentanol connectivity for compound C can be rejected as an option because it is inconsistent with the experimental data: 1-pentanol would have 5 groups of carbons and 6 groups of hydrogens in a 1:2:2:2:2:3 ratio. None of the three alcohols that maintain the five carbons in a straight chain is consistent with the data for compound C, and by following the data, we need to consider the possibility that the connectivity of the carbon atoms has changed. Do not be distracted by how this might take place. *As stated above: You need to figure out what the structure is before you can figure out how it might have been formed, not the other way around!*

Following the deductive scheme used in the prior examples, we start with all the pieces laid out (Figure 0508) and then begin to create clusters of atoms according to the number of groups and their relative sizes.

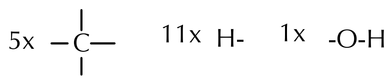
Figure 0508

Deducing the structure of the unknown product from the data in the high temperature hydration reaction of 2-pentene.

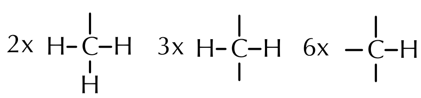


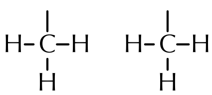
compound A + **compound B** + **compound C**
2-pentanol 3-pentanol
~ 1:1:5 ratio

step 1. the pieces:



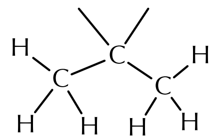
step 2. a set of 6 hydrogens can be





is the only way to do it with this limited set of atoms; 3 CH_2 groups would need to be placed as a single equivalent groups, as would 6 CH groups

2 equivalent CH_3 appear as a set of 6 in compound **B**, but that also required a set of 4 from the two equivalent CH_2 groups, and there are not those in compound **C**, so the two CH_3 groups are on the same carbon atom



step 3. from $C_5H_{12}O$, the set of 6 hydrogen atoms consumed 3 carbons, and the OH group is the set of 1 hydrogen (and the oxygen), which leaves 2 Cs and 5 Hs unaccounted for. With 4 total carbon atom groups, each of these remaining two must be nonequivalent, and there are two more hydrogen atoms groups [2:3 ratio], which means:

step 4. and there is only one way to assemble these pieces (see step 5)

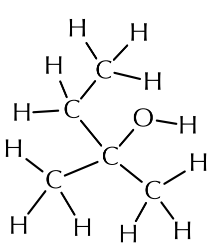
experimental data for compound C

molecular formula: a $C_5H_{12}O$ alcohol

boiling point = 102 °C
melting point = -12 °C
dipole moment = 1.80 D

# of equivalent carbon atom groups = 4
# of equivalent hydrogen atoms groups = 4
ratio of hydrogen atoms is 1:2:3:6

step 5. the proposed structure is consistent with the experimental data about the equivalent and nonequivalent sets of atoms



2-methyl-2-butanol