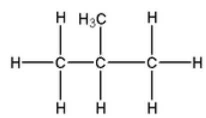
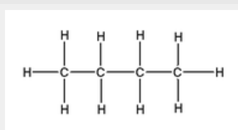
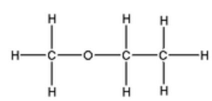
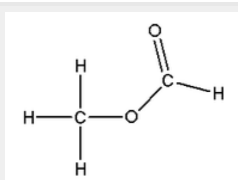
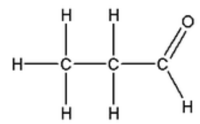
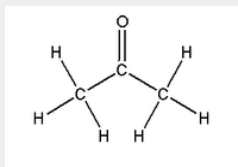
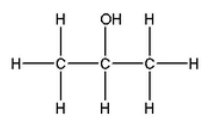
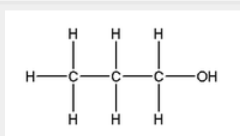
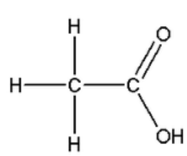
8.17.1: Biology- Entomology

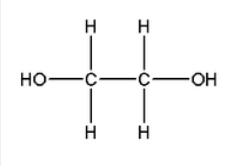
Almost everyone has experienced the stinging of an ant or bee - for some, the reaction is not only mildly painful, but allergic. What causes the stinging sensation, though, is not the initial bite or sting of the insect; a group of organic compounds called carboxylic acids is responsible for the lasting effect. The Southern wood ant (*formica rufa*) can actually shoot a simple carboxylic acid, formic acid, at large distances in self-defense[1] - no stinger needed.

Formic acid, like all carboxylic acids, ionize to release H^+ ions in solution. Why does the (-RCOOH) group define such an acidic compound, when other such functional groups also release H^+ ions? Why do Southern wood ants not shoot alcohol instead of formic acid? This is because their defining functional group is the carboxyl group, (-RCOOH), in which the electronegativity of the two oxygen atoms and resonance of the resulting (-RCOO) anion contributes to deprotanation. In higher concentrations, formic acid can cause liver and kidney damage; however, ant venom is dilute enough to be eventually metabolized by the body, causing the sting to wear off.

The structure of the carboxyl group effects not only the acidity of carboxylic acids, but a number of other physical and chemical properties. For example, hydrogen bonding raises the boiling point of carboxylic acids compared to other functional groups:

Name	Projection Formula	Type of Compound	Boiling Point in degrees C
Isobutane	 "C" "H" 3 group connected to the middle "C" of three carbon straight chain alkane. Left and right "C" is connected to 3 "H" each. Middle C, in addition to "C" "H" 3 group has one bond with "H".	Branched Alkane	-10.2
n-Butane	 Straight chain consisting of four "C". Three middle "C" is connected to two "H" each. Left and right "C" are connected to 3 "H" each.	Normal Alkane	-0.5
Methyl ethyl ether		Ether	10.8
Methyl Formate	 A "C" "H" 3 group is bonded to an "O" which is also bonded to a second "C". This "C" is double bonded to an "O" and single bonded to a "H".	Ester	31.5

Name	Projection Formula	Type of Compound	Boiling Point in degrees C
Propanal	 A "C" "H" 3 "C" "H" 2 group is connected to another "C" which is double bonded to an "O" and single bonded to a "H".	Aldehyde	48.8
Acetone	 Central "C" is double bonded to an "O". Bonded at an angle on its left and right side is two identical "C" "H" 3 groups.	Ketone	56.2
2-Propanol	 "O" "H" group connected to the middle "C" of three carbon straight chain alkane. Left and right "C" is connected to 3 "H" each. Middle C, in addition to "C" "H" 3 group has one bond with "H".	Alcohol	82.4
1-Propanol	 A "C" "H" 3 "C" "H" 2 "C" "H" 2 straight alkane chain is bonded to an "O" "H" group via its last "C".	Alcohol	82.4
Acetic Acid	 A "C" "H" 3 group is bonded to a "C" which is double bonded to an "O" and single bonded to an "O" "H" group.	Carboxylic acid	117.9

Name	Projection Formula	Type of Compound	Boiling Point in degrees C
Ethylene Glycol		Dialcohohl (two OH groups)	198

The extended array of carboxylic acid properties can be made more visible by this JmoL of acetic acid. In the general menu to the left, click on partial charges. Each atom in the molecule will be assigned a partial charge. It is clear that the oxygen atoms are sharing electrons unequally and causing other parts of the molecule to gain a partial positive charge in the carboxyl carbon and hydrogen. Further, this induces a partial negative charge on the methyl carbon, leading to positive charges on the methyl hydrogen atoms.

An even better way to view the electron distribution is with the Molecular Electrostatic Potential (MEP) Surface options. One can look at "MEP on isopotential surface", which show surfaces where electrostatic potential is the same, but the most informative option here is the "MEP on Van der Waals Surface" radio button. This shows the potential along the van der Waals surface of the molecule. The closer to red on the color spectrum, the more negative the potential at that surface is, the closer to blue, the more positive. One can see that both oxygen atoms are centers of partial negative charge, while the acidic hydrogen atom has a substantial partial positve charge, and the methyl group is also has a partial positive charge. One more way to look at the molecule, is to use the "MEP on a plane" button. Choose the XY plane, and then click "Set Plane Equation." This will show the electrostatic potential along the axis of symmetry for the molecule. While two hydrogen atoms on the methyl group are out of the plane, this view still allows one to see how partial charge is distributed along the backbone of the molecule in a way the van der Waals surface does not. From this modeling of the acetic acid molecule, hopefully it is becoming clear how the macroscopic properties we discussed arise.

Pantothenic acid-rich royal jelly.

In entomology, carboxylic acids are not only used for self-defense. Pantothenic acid, $C_9H_{17}NO_5$, is a vital component of royal jelly, a rich honey secreted by worker bees to feed their queen[2]. This compound is not exclusive to bees; pantothenic acid is recognized as vitamin B_5 and is found in many foods, especially in healthily-touted whole grains.

References

1. Educated Earth [www.educatedearth.net]
2. en.Wikipedia.org/wiki/Royal_jelly