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Carboxylic acid vs alcohol ir spectrum

The O-H rack is usually a broad IR band at 3400-3200 cm-1. This is the case if you manage the IR spectrum of the purely liquid alcohol where the concentration is high. Carbon compounds sometimes give rise to a weak C=O overtone at about 2 · 1700 cm-1 = 3400 cm-1. This poor overtone should not be confused with an O-H stretch - an O-H stretch is always strong. Note that the O-H stretch will show up as a sharply weak spike at 3650-3600 cm-1 when the IR spectrum of the alcohol is recorded in dilution solution. At moderate concentrations, the O-H stretch appears both as a sharp, weak peak at 3600-3500 cm-1 and a strong, broad peak at 3400-3200 cm-1. The O-H band of a hydrogen-bound OH is easier to stretch, so it absorbs at lower waveings (Hooke's law): non-hydrogen-bound OH tape (diluted solution in nonpolar solvent) 3650 3590 cm-1 sharp hydrogen-bound OH tape (concentrated solution) 3550 3200 cm-1broad Hydrogen-bound O-H stretches is much broader because the hydrogen bonds vary. Hydrogen-bound OH band 3300 2500 cm-1very broad The difference between the different shapes of O-H stretching is clearly illustrated in the following 3 examples: a) a aromatic alcohol (concentrated sample), b) the same aromatic alcohol in diluted solution (in CCl4) and c) a carboxylic acid (3-chloroponic acid). Note that carboxyl acids of alcohols can be distinguished by the additional, strong carbon rack. The sixth installment in our investigation of the infrared spectroscopy of the carbon group is focused on esters. Like acid anhydre hats and carbox slate, esters are made via a response involving carboxyl acids. Esters are very common and are economically and biologically important. All esters display three intense peaks and therefore follow what I would like to call the Rule of Three. The spectrum of saturated and aromatic esters will be examined over the next two columns. So far in our investigation into the infrared (IR) spectroscopy of the carbon functional group we have looked at ketones, aldehydes, carboxyly acids, acid anhydids, and carboxates (1-5). Acid anhydides and carbox slats are both made of carboxyl acids. If an alcohol and a carboxylic acid are redacted, a functional group called an ester is synthesized. The response is called esterified. My high school chemistry teacher (who was largely responsible for my career choice) helped us remember the name of this response by expressing it ester vacation and saying that was the time off we got from school around Easter. The molecular framework of the ester functional group is shown in Figure 1. Figure 1: The molecular framework of the ester functional group. The carbon in the C = O group in esters is called the carbon carbon, as was the case in all the other carbon containing functional groups we studied The carbon on the left side of the Carbon in Figure 1 is called the alpha carbon, and the oxygen to the right is called the ester oxygen. If the alpha carbon is saturated, it gives a saturated ester, while if the alpha carbon is aromatic, we have an aromatic ester. As we'll see in the next two columns, IR spectroscopy can easily distinguish saturated from aromatic esters. A word about the pronunciation of this functional group is alright. I'm not originally from New England, but I've lived there for a number of years. I observed that the natives loved dropping the r's at the end of words, as excreted in the hacked phrase, Pahk the cahh in Hahvahd Yahd. Not surprisingly, I've heard native New Englanders consistently call this functional group an estah. Esters are industrial and biochemically important. Polysts are important materials made in liquor bottles, dust and clothing. Fat molecules contain a lot of ester liaison. Finally, esters are among the flavorings in food and are used as solvents. The IR Spectroscopy of Esters Note that ester groups contain one C=O band and two C-O effects. We've already studied the IR spectroscopy of both these functional groups, so we can take a stab at predicting what their spectrum might look like. Remember (1-5) that carbon stretch peaks are strong and generally occur between 1800 and 1600 cm-1 (assume that all peak positions noted in this section will be in cm-1 units, even if not explicitly stated). We also know (6) that C-O stretches are intense peaks typically seen between 1300 and 1000. Since one of the C-O tyres in the ester group is attached to the carbon carbon and the other is not, we can expect the two to be chemically clear, have different power constant constants, and thus give rise to two separate peaks between 1300 and 1000. As it turns out, our predictions are correct. Esters have a memorable pattern of three intense peaks at ~1700, ~1200, and ~1100 of the C= O and two C-O stretches, and thus follow what I call the Rule of Three (7). An example of the

spectrum of a saturated ester, ethyl asetate, is shown in Figure 2. Figure 2: The IR spectrum of the saturated ethyl asetate. Noting the Rule of Three peaks labeled A, B, and C. Ethyl acetate is made of acetic acid and ethyl alcohol, one can in theory make it by reacting vinegar with vodka. Ethyl asetate becomes common in food and has a fruity flavor. This is a saturated ester because the alpha carbon is a methyl group. The Rule of Three peaks in Figure 2 is marked A, B and C and is easy to see, stitching like three long fingers in the middle of the spectrum. The peak at 1742, of course, is the carbon stretch, and for saturated esters in general this peak falls from 1755 to 1735. The second peak marked B on 1241 is off the stretch the C-O tape on the left side of the ester oxygen, which is attached to the carbon carbon, and also the stretches of the alpha carbon-carbon C-C band. I call it the asymmetric C-C-O stretch and this vibration is illustrated in Figure 3. Figure 3: The C-C-O rack of the ester functional group. This vibration is responsible for the second of the Rule of Three peaks. In general, for saturated esters this peak falls from 1210 to 1160. The third peak in Figure 2, marked C at 1047, is from the stretch of the second C-O band in the ester, which is the one on the right side of the ester oxygen. This vibration will also involve any carbon attached to the right side of this tape, forming an O-C-C moiety. I call this vibration the asymmetric O-C-C stretch, and it is illustrated in Figure 4. Figure 4: The O-C-C rack of the ester functional group. This vibration accounts for the third of the Rule of Three peaks. For saturated esters in general, the O-C-C-C stretch appears from 1100–1030. To be clear, a linkage like C= Oh (O-CH3), which has an O-C tape rather than an O-C-C moiety, will still exhibit this peak. If you carefully reread this section, you might note that I lied to you. I said above that to saturated esters that the C-C-O stretch falls into the 1210-1160 series, and yet clearly the C-C-O piece of ethyl asetate falls at 1241. What's going on here? This spike is definitely a rule exception, but for once it's one we can understand and use of. Asetate esters are unique in that the alpha carbon is just a methyl group with nothing else attached. Remember from the first installment in this series (8) that one of the things that determines peak positions in IR spectroscopy is mass reduced, and that if the reduced mass of a functional group measured its IR peak positions in wavenumber. A methyl group is all about the lightest alpha carbon you can have in an ester, which is probably why asetate esters have a uniquely high wavenumber C-C-O stretch that typically falls around 1240. Acetate esters are common due to the ubiquity of aset acid. The fact that they have a unique asymmetric C-C-O stretching peak is useful in discriminating them from the many other types of saturated ester. Note in Figure 2 that as we go from left to right to peaks A, B and C, the third peak is a little less intense than the other two. This intensity pattern is typical of esters and can be useful in identifying them. A summary of the group of wavenumbers for saturated esters is found in Table I.Conclusions Esters is a common and economically important functional group made by reacting to an alcohol and a carboxylic acid. Their structural framework consists of a C=O group and two C-O effects. This gives rise to three intense peaks called the Rule of Three with peak positions at about 1700, 1200, and 1100 wavenumbers. The three vibrations is the C=O stretch, a C-C-O rack, and an O-C-C-C rack. Saturated esters were here, aromatic esters will be covered in the next installment.

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