Multi-Spectrum Analysis

Transcript

00:00:00:00 - 00:00:08:68
Dr.Jessie Key: So again, Dr. Jessie Key here. In this video, we are going to see how we can use multiple spectra to help identify an unknown compound.

00:00:08:68 - 00:00:46:47
Dr.Jessie Key: For this example, we are told to use the following spectra to determine the identity of an unknown compound with molecular formula C9H8O2. We can use the formula learned in CHEM 2123 to help us determine the degrees of unsaturation in the molecule. So our formula for degrees of unsaturation is two times carbon, plus two plus N minus H minus X, all divided by two.

00:00:46:47 - 00:01:34:31
Dr.Jessie Key: Now let's put the values from the molecular formula into this equation. We have two times nine, plus two, plus zero, minus eight, minus zero, all divided by two. When we do the math here, we end up with six degrees of unsaturation, having four or more degrees of unsaturation is often a sign that there's an aromatic ring present.

00:01:34:31 - 00:02:01:27
Dr.Jessie Key: In this case, having six tells us that there is likely an aromatic ring and two additional Pi bonds or rings. This will help us deciding on the structure of the unknown. Starting with the IR spectrum, we can identify that there's a carboxylic acid present by its characteristic broad, un-uniform O-H stretch signal ranging from 3500 to around 2500 wavenumbers.

00:02:02:85 - 00:02:40:45
Dr.Jessie Key: A C double bond O (A C=O) stretch is present at 16 73 wavenumbers (cm-1), which supports the presence of a carboxylic acid. In addition, there's a pair of signals corresponding to CC double bond (C=C) stretch 1650 and 1400 wavenumbers (cm-1) and a possible sp two CH (sp2 C-H) stretch signal poking through the O-H stretch at 3065 wavenumbers (cm-1). This suggests the presence of alkenes and/or aromatics in the molecule.

00:02:40:45 - 00:03:00:53

Dr.Jessie Key: Looking at the proton NMR spectrum, the broad singlet at approximately 11.5 ppm suggests the presence of a carboxylic acid proton. There are seven protons worth of signals in the aromatic region, suggesting that we have an aromatic ring and something else fairly deshielded.

00:03:00:53 - 00:03:21:01
Dr.Jessie Key: The multiplet signal integrating for five suggests that we have a monosubstituted aromatic ring, as these will often appear as multiplets like this on lower resolution NMR instruments. The two doublets, integrating for one each at 7.6 and 6.5 ppm suggests the possibility of an alkene.

00:03:21:01 - 00:03:55:54
Dr.Jessie Key: There are no significant peaks further shielded in the spectrum, which suggests the absence of any alkyl groups. Looking at the carbon MMR, the signal at 168 ppm supports the presence of a carboxylic acid carbon. The signals 150-125 ppm are in the range for aromatic carbons, there's a single signal at ~120 ppm which may correspond to an alkene carbon.

00:03:55:54 - 00:04:24:51
Dr.Jessie Key: Putting this evidence together suggests the following structure. Note, it is important to double check the degrees of unsaturation and the molecular formula match after proposing a possible structure. There are four degrees of unsaturation from the benzene ring, one from the alkene and one from the carboxylic acid pi bond.

00:04:24:67 - 00:04:30:55
Dr.Jessie Key: This checks out with our previously determined six degrees of unsaturation.