CATHERINE DRENNAN: Lewis structures. So I tell students who have sort of no background in chemistry before they come into this class, and there always are some, that there are some topics in 5.111 that having no experience with the topic is actually a good thing, and Lewis structures is one of these things. I think if you've seen it before, you're like, oh yeah, that's easy. I know how to do that. You don't practice and you get on an exam and you're like, oh wait a minute. I forgot how to do this.

And the students who haven't seen it before know all the rules and just get brilliant, perfect scores on the exam. And the other students are like, man. I forgot how to do my Lewis structures. So here are Lewis structures. We're going to go over them. So I really like Lewis structures because they're relatively simple, and they work. Like 90% of the time, they are the correct structure. And I'm a big fan of simple things working.

If you wanted to get from 90% to 100%, you'd have to use Schrodinger's equation, but you can get 90% just with the simple Lewis structures I'm a big fan of that. I love it when simple things really work pretty well. OK. So when Lewis structures the key to this is thinking about the electrons being shared so that you get a full valence shell. And having the electrons distributed in such a way that all of the atoms have the number of electrons that make them happy, which is usually eight electrons, which is an octet, that noble gas configuration.

So every dot in a Lewis structure represents a valence electron. And we can then look at some atoms and put dots around them to indicate the number of valence electrons. So we also have to know how many valence electrons atoms have. And so why didn't you just practice with a clicker question. And here's part of the periodic table up here if you need it. All right. I'm told 10 seconds. Everyone was crazy fast. Yes.

So seven is the correct answer. You could look at the periodic table and sometimes with these it's a counting thing. So this is one where you want to always double check if things don't make sense. All right. So we can put seven electrons around fluorine, and we'll have two fluorines here. They'll both have seven electrons around them. And now I'm going to jump to another slide, but I'm going to show you the seven again in case you haven't written them down. If you don't want to, they're not in your handout, but that's probably OK.

So when you bring them together, you can bring them together in such a way that they can all share. And so if we put in green, then, one of the fluorine's seven. And then we put in blue the other fluorine's seven, you can see that they can share two in the middle and both are very, very happy. So just thinking about this really simple idea, how many electrons will give you an octet, will give you eight? And how can you put things together in such a way that allows for that to happen?

Now there are a few elements that do not want eight in their valence shell, and hydrogen is one of them. It just has that one S. So it only wants two, that's all it can handle. So this is an exception, hydrogen is going to want two electrons. Hydrogen loves to interact with things, though. It interacts with lots and lots of things. And here hydrogen with its one valence electron is interacting with chlorine with its seven valence electrons, and they are sharing two electrons forming a bond together.

So when we're talking about Lewis structures, we're talking about different kinds of electrons. So we're talking about bonding electrons, the electrons that are involved in the bond, and also lone pair electrons. So chloride in HCl is going to have two bonding electrons, one was its, and one came from hydrogen. And it's also going to have six lone pair electrons, or we could say three lone pairs. So when we say a lone pair, that indicates two electrons there. So it has one, two, three, four, five, six or one pair, two pairs, three pairs.

Now there are rules to Lewis structures, and here is the complete rule. In your handout, this wouldn't fit on one page. It's on two pages. And these rules, if you do work these problems, you will remember these rules, and they become pretty easy. But it's important to work Lewis structure problems so that the rules become really familiar to you. And it takes time to work Lewis structure problems, so don't wait to the last minute to start this problem set. There's a lot of Lewis structure problems on it, which means it's not difficult, but it's going to take some time.

All right. So let's briefly go over these rules. First what you want to do is draw in the skeleton structure. Just put the atoms down. Hydrogen and fluorine are always going to be terminal atoms. Don't put them in the middle of a molecule. That gets chemistry professors really upset to see hydrogen in the middle with lots of bonds to things, so don't do it. And typically the element with the lowest ionization energy goes in the middle, and there are some exceptions and we'll see some of those exceptions. But that should be your first guess.

You want to count the number of valence electrons. If there's a negative charge, you need to count that in or if there's a positive charge you need to subtract that from the total. Then you want to figure out the total number of electrons needed, so everyone has their full valence shell. You need to subtract these two to get the number of bonding electrons. And here are some of the things that it's really easy to make math mistakes here, so if your structure makes zero sense at the end, go back and check your math. Assign to bonding electrons to each bond. If any remain, you want to think about whether you have double or triple bonds.

And there's only certain kinds of atoms that can have double and triple bonds. So be careful where you're putting your double and triple bonds. If any valence electrons remain, those are loan pairs. And then lastly, you want to figure out the formal charge on all of the atoms in your structure to make sure that this is a valid structure, and we're going to talk about formal charge. So first, let's just try an example. And your sheet has two examples on the same page. We have HCN and we also have CN minus.

So we're going to do HCN first, so don't fill your entire page because you're going to have to write things for CN minus as well. But before we start, we need to figure out which atom is likely going to be in the middle. And so why don't you tell me what you think on the clicker question. OK, 10 more seconds. Yup. So here again we want to have one that has a lower ionization energy, and you also want to consider other things like hydrogen can't be in the middle.

OK. And it was written that way, but sometimes they're written in a way that is not as straightforward. OK. So I'll put that up. All right so we'll go through the rules and we'll try to work this out. So first I can write-- I'm going to start-- I guess I'll write over here. So number one, we're just going to write HCN with C in the middle. So that's the first thing we're going to do. Next we're going to consider the valence electrons. And you can just help me out by yelling things out.

How many valence electrons does hydrogen have?

AUDIENCE: One.

CATHERINE What about carbon?

DRENNAN:

AUDIENCE: Four.

CATHERINE DRENNAN: Nitrogen?

AUDIENCE: Five.

CATHERINE DRENNAN: And you can always check me on my math. How much does that equal?

AUDIENCE: 10.

CATHERINE DRENNAN: Excellent. There's nothing like adding simple numbers in front of 350 people to really put the stress in one's day. OK, so to have a complete full valence shell, what do I need for hydrogen?

AUDIENCE: Two.

CATHERINE DRENNAN: What about carbon?

AUDIENCE: Four.

CATHERINE DRENNAN: Eight to be complete. Nitrogen?

AUDIENCE: Eight.

CATHERINE DRENNAN: Eight. And I think we add this up, we should get 18. How's that? All right. So for four, now we're going to subtract these numbers from each other to tell us how many bonding electrons we have. So we have 18 minus 10. And we should have eight to bonding electrons. For five I'm going to now assign two per bond. So I'm going to put one here. Another here. Another here. Another here. So I've assigned two per bond.

And now I see if I have any left. Do I have some left? I've used four, I had eight. So yes, I have four more. And if you have more bonding electrons, then you are supposed to assign those bonding electrons. And think about whether it's allowed to have double or triple bonds. Can hydrogen be involved in the double bond? No. Carbon nitrogen?

AUDIENCE: Yes.

CATHERINE DRENNAN: Yes, or a triple bond. So I have four more, so I'm going to put one, two, three, four. So I'm going to have a triple bond between my carbon and my nitrogen. And now I'm good. So now I want to see do I have any extra electrons. So for this, I had 10, I used eight, so I have two left. So I'm going to assign those two as a lone pair. Should I put them on hydrogen? What about carbon? No. Carbon already has its eight, because it has four bonds. So then I'm going to put it on nitrogen.

And then the only thing left is formal charge, which we haven't talked about yet. So before we do formal charge, I just want to do the same thing with CN minus. And I will say if you want to draw triple bonds, that's fine too. You don't have to indicate the dots as bonds. It's perfectly fine to write out a triple bond. So I could have written this as well. OK, so let's look at CN minus. So how many valence electrons does carbon have again? Four. Nitrogen? Five. Am I done?

AUDIENCE: No.

CATHERINE DRENNAN: No. I need to add one because there's a charge on this molecule of minus one. So now so I have 10 again. Three I'm going to figure out how many electrons I need to complete my valence shell. How many from carbon?

AUDIENCE: Eight.

CATHERINE DRENNAN: Eight. Nitrogen? Eight so now I have 16. I will subtract. Now 10 from 16 and get six bonding electrons. And I'm going to assign first just two of them. So I'll assign one, two here. And then we-- this is to assign. Six said, do you have any left over? I had six, and I only used two, so the answer is yes. I have four more. So I can put those in one, two, three, four.

Again, we're going to have a triple bond. And then we ask are there any electrons left? So we had 10, we used six of them. And so we're going to have now four more here. So now I can assign-- this only has-- this is not complete for carbon. So I can put a lone pair on carbon, and I can put a lone pair on nitrogen. And now they have their complete octet. And we get to assign formal charge. So I could write it this way, or I could have written it with a triple bond here. And don't forget to put the charge on the end.

All right. So now let's consider formal charge, because we're never done with our Lewis structures until we've considered formal charge. So formal charge is a measure of the extent to which the atom has really lost or gained an electron in the process of forming this covalent bond. So as we'll talk about, it's not the same as oxidation number where you have like sodium plus one, but again, there's some differences in how many are brought to the table and what it ends up with in the end.

So there's an equation which you'll have to learn, but if you do enough of these problems, it'll be stuck in your brain and you can't purge it even if you want to. And so formal charge, FC, is equal to the number of valence electrons, symbol V, here, minus the number of lone pair electrons minus half of the number of bonding electrons. So at least this equation makes sense. If you forget what they mean, you can probably think about it and it'll come back to you.

So in doing these formal charges, you want the formal charges to add up to the charge on the molecule. So if we had HCN, that's a neutral molecule so the sum of all of the formal charges must be zero or you did something wrong. If it's CN minus, the sum of the formal charges has to add up to minus one or you did something wrong. So this is a good way of checking your math. So always remember that the sum needs to add up to the total charge on the molecule. If you remember that, that's a really good check to make sure you didn't make some kind of weird math mistake and add things wrong and have an appropriate number of loan pairs or something going on.

OK. So let's calculate formal charge now on our CN minus molecule up here. So the formal charge now on carbon here. So how many valence electrons do carbon have?

AUDIENCE: [INAUDIBLE]

CATHERINE DRENNAN: Four. How many lone pairs does it have?

AUDIENCE: [INAUDIBLE]

CATHERINE DRENNAN: It has one lone pair, two lone pair electrons. This is the total number of lone pair electrons here, and then half the number of bonding electrons. So it is expanding electrons and half of that is three. And so that should add up to a charge of minus one. You can also, instead of thinking half the number of bonding electrons, you can also just think about number of bonds if you want to to do this.

All right so to see if you have the hang of it, let's do a clicker question. OK, 10 more seconds.

Most people got it right. I can't actually read the number, but that was very good. It always seems wrong to put zero as the answer, but that is, in fact, the answer here. So if we look at this again, we have five valence electrons on nitrogen. We have two lone pair electrons, and we have six bonding electrons. Half of six is three, and so that's zero.

Or you could have said, well, if this is minus one, and the charge is minus one, then that had to have been zero, otherwise Professor Drennan did something wrong, and that's just not possible. So the answer there would be zero. And you can see that the total formal charge is minus one, and the total charge of the molecules also minus one. So again formal charge does not equal oxidation number, it's something special. It tells you kind of in this arrangement of atoms in the molecule, did this atom kind of come up with a little bit more at the end or a little bit less, depending on where it started from and where it is. And where you want in these structures for the formal charge to be low.

So we can use a formal charge to decide between Lewis structures so that the structures with the lowest absolute values of this formal charge are more stable structures. So if you have really high formal charges, that means that molecule isn't really very stable because you want low charges. You want lower energy. You want things to be in a more neutral and happy state. So we want to figure out which ones are going to have low charges.

So let's look at another example, Thiocynate ion, and it has a carbon, sulfur, and nitrogen in it, and it has a charge of minus one. So I might tell you the ionization energies for carbon, sulfur, and nitrogen, and then ask you which atom do you think is going to be in the center of the molecule? So what do you think? What's in the center of this molecule based on those numbers? Just yell it out.

AUDIENCE: [INAUDIBLE]

CATHERINE DRENNAN: Sulfur. So sulfur has the lowest ionization energy, and I told you that's usually the thing in the center. But you can start with that. It's always good to start with that, but then you want to check the structure and make sure that a structure with sulfur in the middle has the lowest formal charge. So let's take a look at that. So we can draw structure A with sulfur in the middle, and then calculate the formal charges on that.

And if we do that, we see for the nitrogen here, nitrogen has five valence electrons, it has four lone pair electrons, and it has half of four bonding electrons, so it would have a formal charge a minus one in this particular structure that has sulfur in the middle. We can look at carbon.

Carbon has four valence electrons, Four lone pair electrons, and half of four bonding electrons, so it has a charge of minus two. Then we can look at sulfur. Sulfur has six valence electrons, zero loan pairs, and half of eight bonding electrons, so it has a formal charge of plus two.

So overall, this does equal the minus one. So it's a valid structure. But is that the lowest energy one? We also could put carbon in the middle or nitrogen in the middle. So let's look at what this does for us. So with the formal charge on nitrogen now, we have five minus four lone pair electrons, minus half of four bonding electrons, minus one. So that's the same. Now we can look at carbon. We have now just no lone pair electrons. It has four minus zero minus four, half of eight bonding electrons, or zero. And for sulfur, six minus four lone pair electrons, and half of four bonding electrons, or zero.

Next, structure C, five minus zero lone pairs minus half of eight, plus one. So that one's different. Carbon, we have four valence electrons minus four lone pairs minus half of four, bonding minus two. And for the sulfur, six minus four lone pairs electrons, half of three or zero. So now with the clicker, tell me which is most stable. All right, 10 seconds. I think this can be 98%. That's what I'm thinking. I'm feeling good. Well, close. Yeah. What? No, no. Sorry.

It should be B. Yeah, it should be B. Yeah. Sorry I actually-- Yay. There we go. Yeah, B is correct. So if we just look at it over here, it has the lowest number of formal charges, so the answer is B. OK. Let's start with this simply. Who wants to tell me why one, how they could look at this and realize one was not the correct answer? I think this is on. Give it a try.

AUDIENCE: One's not correct because if you look back at your atomic radius chart, this is pretty much doing the exact opposite of that

CATHERINE DRENNAN: Yeah, so helium definitely not the biggest atom there is. OK so six got a lot of attention, and so did two. And ionization energy, electron affinity, and electronegativity are definitely connected to each other, but there is a clue that electron affinity would not be the correct. Does someone want to say what you might have noticed?

AUDIENCE: For electron affinity, it increases and then stops at the noble gases because noble gases do not want electrons. So in this particular chart, all the noble gases are like the highest-- are the highest ones in the relative area, which would mean that electron affinity would be incorrect.

CATHERINE Yep. That's right so the noble gases were the clue. So [INAUDIBLE]. Yep. And so if electron

DRENNAN: affinity also is not high at the noble gases, they're also not electronegative. Noble gases just don't want extra light. They don't want to lose electrons, they don't want to gain electrons, they just want to be left alone. So this trend is for ionization energy. And because noble gases want to be left alone, they don't want to lose any of their electrons.

Great. So this is good to be thinking about, because we're finishing up now for the handout from last time. And we're going to be talking about electronegativity again. We never move very far away from a lot of these topics. They just keep coming back. So we just keep reviewing them. All right, I don't need to microphones, although, I don't know, I kind of like having this one. Anyway. So let's take out the handout from last time, and let's finish it up.

We were talking about formal charge, and we had looked at examples where we calculated formal charge, and then we looked at which structure would be lowest in energy, and that was the structure where you had the least separation between the charges on them, so the smallest absolute numbers. If you have formal charges of zero, that's fantastic. That's what the molecule wants. Minus one, plus one, if you must, but when you start having plus two minus two, that's a lot of charge separation, so that's less favorable.

So we're going to have more examples of that as we go along. But now, what-- if you had calculated formal charge and they're all the same, how do you know which structure is correct? So what if you have-- and this is-- just some people who are having trouble. This is the top of page four from the handout. You have two valid Lewis structures that have the same formal charge, how do you know where it goes? And the answer is that the negative formal charge should go on the most electronegative atom.

And so that's why we are sort of talking about electronegativity again. And so electronegativity-- remember electronegativity is high when the electron affinity is high, meaning that the atom wants to get an electron, has a high affinity for electrons, and also a high ionization energy, which means it doesn't want to give up its electrons. So that's something-- it likes to have electrons, and so you want to put a negative value, which indicates there's more electrons on something that's electronegative. So negative on negative over here. And so that's what you're looking for. That's how you're going to make a decision.

So let's look at an example. So here is a molecule, and we're going to look at two possible Lewis structures of this with similar formal charges, and decide which has the correct structure. So first let me give you a couple hints that can be useful in problem sets and in exams. When you see CH3, that's a methyl group, and that's going to be terminal so you're going to have these three hydrogens associated with that carbon, and that's going to be at an end of the molecule. So it could look like one of these two things.

So we have the carbon, we have it attached to three hydrogens, a carbon attached to three hydrogens, and then attached to something else, this nitrogen here. And this structure where it's just kind of written out in a line or a chain of atoms, what we call chain molecules sometimes. Often the atoms are actually written in the order in which they're attached, so that's definitely true here. CH3, three hydrogens attached to the carbon, so they're attached to the atom that came before in the chain.

The nitrogen is also going to be attached to the carbon. Even though it follows the hydrogen, you're not going to have hydrogen in the middle of a bond. It's not going to be bonded to two things. Hydrogen is always terminal, so even though nitrogen is here, it's got to be attached to the carbon. So we have three hydrogens and then a bond between the carbon and the nitrogen. Now we have a hydrogen after the nitrogen, and by this rule it should go on the nitrogen. But you might want to double check that that's true. And then we have an oxygen. Again, the oxygen is going to have a bond with the nitrogen. You're not going to have a bond with hydrogen in the middle. Hydrogen's always terminal.

So the only real choice we have here is we can put the hydrogen on nitrogen or we can put the hydrogen on the oxygen here. And so we can use this rule about electronegativity and formal charges to figure out which of these structures is right. So in this particular case, all of the formal charges are zero on all of the atoms, except there's one minus one charge. And in this structure, the minus one charge would be on the oxygen, and in this structure the minus one charge would be on the nitrogen.

And if everything else is zero then you have the sum of your formal charges, minus one, equal to the charge on the molecule, which is minus one. So both of these are valid structures. Both have low values of formal charge, which is right. So it's going to be the structure that has the negative charge on the most electronegative atom is the right structure. And so here you need to remember some of your rules about electronegativity.

And in terms of electronegativity, we see that oxygen has greater electronegativity than the nitrogen. And so that's where we would want to put our negative charge-- on the negative charge goes on the atom that's the most electronegative. And that would generate the lower energy structure. So if you're given a table of electronegativities, which you often are, you can look it up and validate that that's going to be the correct place. And in fact, experimentally we know that that's the right structure. So that works. So if you have two structures, identical formal charges, valid structures, then the last step is to think about where that negative charge should go, and pick the atom that is the most electronegative.

All right we have one more thing we need to talk about in Lewis structures before we start violating various rules that we've learned, and that is that we need to talk about resonance structures. And so to explain to you what a resonance structure is, it's really helpful to start with an example, so that's what we're going to do. And we're going to consider ozone, which is three atoms of oxygen. And we have the ozone layer, which protects us from UV damage and is very valuable, and we should not destroy it with chemicals being released into the environment. And because you don't have complete say over that, always wear sunscreen. OK.

So let's build up these Lewis structures, and then consider what's meant by a resonance structure. So here we have part of the Periodic Table that you're going to need, and we need to think first about the valence electrons. So oxygen has six valence electrons and there are three oxygens, so that's 18. To get a full octet for each of the oxygens, three oxygens, an octet is eight valence electrons, so that would be 24. To figure out the number of bonding electrons, we're going to be subtracting our octet electrons from our valence electrons. So 24 minus 18 is six.

And then our next step is to assign those bonding electrons two at a time, two per bond. So let's take a look at that. We can put one bond here between these two oxygens, one bond here between these two oxygens, and then ask do we have any more? And we do. Because we have six bonding electrons, we used four, so we have two more bonding electrons. So we need to make a double bond. But now we have the question of where to make that double bond. Am I going to put it between these two oxygens or am I going to put it between those two oxygens?

And so I could say put it there, but I could also, in structure two, put the double bond over here. All right. We'll come back to that question in a minute. Let's first figure out if we have any remaining valence electrons, and we do. So we had 18 and we've only used six, so we have 12 left. So we're going to put those in as lone pairs. And so I can put them in over here. One set here, one, two, three, four, five, six. And I can also do that over here. One, two, three, four, five, six. And now we have two structures, so we need to think about formal charges to see if that can help differentiate structure one from structure two.

OK. And let's look at that. Be sure everyone's ready. And that is a clicker question. So I'll put that back up. All right. Let's just take 10 more seconds, and we'll talk about what the right answer is, and a little bit of a trick for doing these, perhaps, a bit faster. OK. So that was pretty good.

So let's look at why that's the right answer. And we'll take a look at that over here. So let's do the calculations. So you have to remember the equation for formal charge for sure and once you do enough problems it should stick in your head pretty easily. So if we look over here-- so this is the formal charge on oxygen A. There were six valence electrons, there are four lone pair electrons, minus half of the bonding electrons. There are eight bonding electrons, so that's two. So that's a formal charge of zero.

For oxygen B over here, we again have six valence electrons, and we have two lone pair electrons. We have six bonding electrons, so half of six is three, which is plus one. And on oxygen C over here, six minus six lone parallel electrons, half of one bond, so half of two is one, minus one, overall the charge here is neutral. And that's good because it's a neutral molecule. So to do this structure faster, you have to realize that oxygen A over here is the same as C over there. So you can just copy down what you had for C is now A. B is exactly the same in the two structures, so it's the same as what you calculated.

And now this C was the same as this A, so we can put that same value that we calculated for A into C. So they're both the same. Same formal charges, which structure is correct? And the answer is both of them. And in fact, you need both of them, so there's data-- chemists love data-- and the data is that the bonds are actually equivalent in the molecule. So it isn't that there's one double bond and one single bond, there's just one kind of bond in ozone, and it's between a single and a double bond.

And so this is how one would draw that kind of thing. You would have structure one here and structure two here. You would put them both in brackets, and you would put this special double headed arrow between them and that indicates that both of these structures are needed to describe the properties of the molecule. You do not have a stationary double bond and a single bond. You have kind of a mixture between these two, and that's what a resonance structure is.

So let's take a little bit more of a look at this. So this is just what I had before, experimental evidence is that the bonds are equivalent. There isn't a double and a single, there's something in between, a one and a half. And this is called a resonance hybrid, and it's of length of these two structures. So this structure is blended with that structure. So some of you are aware of hybrids from biology, and now with cars. So a mule would be an example.

And if you're thinking about what a mule is, you don't walk out into your barnyard one day and see a donkey one day and you go out the next day and you see a horse. A mule is a hybrid between a donkey and a horse. So if you were a chemist, you would do this. You would put the donkey in brackets, and the horse in brackets, and put your double headed arrow. And if you see this, you'd say, oh yes, a mule. So that is what this is. Both structures are needed to describe ozone. One structure isn't enough. You need both of them. They're in resonance with each other.

And so what's true about the electrons in ozone is that they're delocalized across all of these bonds, so there isn't like a double single. All of those electrons are delocalized. They're shared over this set of atoms. And you can have two resonance structures, you can have three, you can have four. It depends on the molecule in question. And in all those cases, those electrons would be delocalized.

So just to sum that up, resonance structures, two or more, same arrangement of atoms-- and that's important. It's the electrons that are different. And this isn't in your handout, out but just think about this for a second-- because it was in your hand out a minute ago. Are these resonance structures? No. They're not resonance structures. The atoms are in different positions. So one of these structures is right one of these structures is wrong. With resonance structures, they're both correct and both needed to define the structure. So pay attention. This is a common mistake. Pay attention. Ask yourself, are the atoms in a different position? That's not resonance. You're just looking-- atoms are the same, formal charge are the same, you're just looking at whether you have different arrangements of electrons.