SAL: Hi. I'm Sal. Today we're going to be solving problem one of exam three of fall 2009. Now before you attempt the problem, there's a couple of things that you should know or have background knowledge of these materials before starting. First thing is understanding the properties of crystal defects and for this problem particularly, Frenkel defects, which we'll talk about. The formula, which is an Arrhenius relationship, as a function of temperature and energy enthalpy of the fraction of vacancies that are formed in a crystal and the conversion again between one electron volt and to the joule. This will help you solve the problem. So the problem reads as follows.

Silver bromide, which is AgBr, has rock salt crystal structure. So it's an FCC Bravais lattice with the ion pair Ag plus and the Br as the basis-- Br minus the basis. The dominant defect in AgBr or silver bromide is the Frenkel disorder. So it's telling you what the dominant defective is.

So the question asks, for part A, so I'll put A here. Part A for the question asks, does the Frenkel disorder in silver bromide create vacancies of silver plus, vacancies or Br minus or both? Explain.

Dionic radii are 0.67 Angstroms for silver plus and 1.96 Angstroms for bromine minus. So that's data that's given to us. I'm going to go ahead and write that down.

So I know from reading about point defects and crystals that a Frenkel defect is pretty much formed when you have an ion pair of dissimilar sizes. So if one of the radii-- like, say, your anion is a lot bigger than the radius of your cation, then one should expect that you would have a Frenkel defect to form. And what a Frankel defect is-- which you should know from reading the material-- is that it's when one of the ions in your crystal leaves and leaves back a vacancy-- so just migrates-- just hops out of its lattice site and leaves back empty spaces, which is called a vacancy.

So we're given two things. If I draw a little picture-- I can call this my silver and I'll call this my bromine. And I'm given the fact that the radius of Ag plus is equal to 0.67 Angstroms-- and an Angstrom is just 10 to the minus 10 meters-- very small number. And I'm also given the radius of bromine, the anion, is 1.96 Angstroms. Now I would argue that these two have very dissimilar radii. Obviously, the bromine looks to be about three times bigger than your silver. So by understanding the definition of a Frenkel defect, I can claim that I would expect the smaller ion of the two to be the one that leaves the vacancy behind, hence forms the Frenkel defect.

So for part A, do I expect it to create silver plus vacancies or Br minus vacancies or both? I would expect just to be silver plus, given the size of your cation. So if you were to write on this problem, just expect only Ag plus, which is your silver cation, or the smaller one. Expect Ag plus smaller ion to create a vacancy and hence, this leads to the Frenkel defect.

So yes, I should expect it to form a defect now. If I was given a cation that had a similar radius that I-- I wouldn't know if I could argue the fact that this will form a Frenkel defect or not because the conditions are that you have to have the similar radius between your cation and your atom-- and it makes sense because the fact that your silver is small-- it has more freedom to hop around. So it requires less energy for this smaller atom to then start hopping around your lattice site without penalty or without major penalty compared to your bromine ion. So therefore, this is the one that should be expected to form that. OK. So that's part A.

And part B reads-- calculate the temperature at which the fraction of Frenkel defects in a crystal with silver bromide exceeds one part per billion. The enthalpy of Frankel defects and formation, delta h sub f, has a value of 1.16 electron volts per defect. And the entropic pre-factor A has a value of 3.091. So it's giving you data.

Now the way I would solve this problem is that the first thing I would do is that I would write down what my data is. So I'll call this data and the first thing is that our fraction of vacancies that are formed in silver bromide is one part per billion-- so 10 to the -9. That's a fraction so no units.

The second thing that we're given in the problem is that our energy of formation-- our enthalpy energy-- is 1.16 electron volts per defect. This is the energy penalty for every time one of your silver cations jumps out of sight to create that. Nothing is free. Everything requires energy. We're also given the fact that A, the entropic pre-factor, is 3.091-- with no units-- and given our equation that I showed you on the bullet point. That you should know-- you can go ahead and see what's missing.

So if I write down my equation-- this is all-- I'll box this off as my data because I'm going to refer to this to solve the problem. And the problem talks about temperature. So I know that f sub v is going to equal to the pre-factor times the exponent of negative delta h, of formation over kb t. Now you notice that kb wasn't given to you and kb is both in its constant.

Now a lot of student forget that they have a table of contents in front of them and that value is in there. So if you don't know it by heart, then you want to make sure that you reference to that table because a lot of information will be given to you, because you're expected to look at the table of contents or your periodic table. But if I include this as my data-- I'm going to go ahead and write it over here-- that kb-- half the value of 1.38 times 10 to the -23 and this has units of joules for degree Kelvin. So this is something that you should pay particular attention to because now kb is in joules for Kelvin, but our energy was given in electron volts. Now this is the number one thing that will take off points. You'll get points taken off if you don't notice this-- that you need to go ahead and do the conversion from electron volts to joules or joules to electron volts. Either which way, you're going to get the answer.

But the problem asks, calculate the temperature. The very first sentence. So what does that mean? Well, I'm going to go ahead and look at my equation and I'm going to look at the data that I have and the constants and see if I'm missing anything else because obviously you can't solve an equation that has two unknowns and just one equation. Solve the equation, you've got to only have one unknown for the equation. So f sub v-- no. Check-- no. That's given. Is A given? It's right here. That's given as well. What about delta A sub F? Well, that's the energy-- the energy penalty to create a defect and kb, which we got from our table of contents, and t. So this concludes that the only thing we're not given is temperature because that's what we're asked to solve.

So I need to do some math on here to go ahead and solve for temperature. And the first thing I want to do is take the natural log of both sides. So by taking the natural log of both sides-- so natural log of f sub v-- this equals to natural log of A plus the natural log of the exponent part and we know from math that the natural log of an exponent cancels each other out because they're inverses. So the natural log of exponent, of negative delta h sub f, over kb t-- this cancels that and we just get the natural log of A plus negative because you have a negative up here-- delta h of formation divided by kb t.

So the only thing we don't know here is temperature. So if I can rearrange this equation and solve for temperature, I can get an answer. So if I do that-- what's the best way of doing that? Well. I can add-- I can move this to the other side and move this to the other side and that gives me delta h sub f divided by kb t equals natural log of A minus natural log of your vacancy fraction and I can then multiply both sides by t so it cancels this one and it arrives over here and then divide both sides by ln of this. So I'll go ahead and do that. So I'll multiply this by t. Multiply that by t. So that cancel that and I end up having delta hf over kb t-- the t got canceled-- this equals to the natural log of A minus the natural log of your vacancy fraction times t. So now if I divide both sides by this factor, I solve for temperature. So this gives me an isolation that t ends up being delta hf over kb times the natural log of A minus the natural log of the vacancy fraction. Now all we have to do is plug in the numbers, but again, if you look at the units of Boltzmann's constant, which are joules per Kelvin and the value that we're given up here is electron volts for defect, we want to go ahead and convert the electron volt to the joule because it'll just be easier to do the math that way. So I can go ahead and write it out and I do that by multiplying the top by that conversion factor and if I do the math, t ends up being-- we have 1.16 of this-- has units of electron volts for defect and then I want to get joules because that's what Boltzmann's constant has. So in order to get joules, if I multiply this by the conversion factor which is 1.6 times 10 to the -19-- this has units of joules per electron volt. Now the electron volts cancel and I get-- the numerator has units of joules per defect. That's good because that's going to cancel with the units in Boltzmann's constant.

And then I put in 1.38 times 10 to the -23-- this is joules per Kelvin-- and this factor is multiplied by the natural log of 3.091 minus the natural log of 10 to the -9. So unitless-- so if you do the math out, you end up getting a value that at the end of the day, your temperature-- this t right here-- will be equal to-- let's go ahead and write it over here.

So now that we go ahead and do the math-- that way it's nice and clean. We know that the t, the temperature that we got from plugging all that math-- ends up being just 615 Kelvin. And where did the Kelvin come from? Well, it came from your joules per Kelvin, from your Boltzmann's constant, because that's what the dimensional analysis does.

So this is the answer. This is good. The problem doesn't say show the answer in degrees Celsius, but since everybody knows degrees Celsius-- everybody in science relies on degrees Celsius-- you can just convert this over to degrees Celsius, which happens to be 342 degrees Celsius. So this right here is your answer to part B.

And again, I want to express again that the crucial part in getting this is knowing the fact that you're given an energy in electron volts, but the constant that you use has units of joules. So you need to convert to get the right unit out or else you will get not Kelvin-- you would get something different here, which wouldn't make any sense given the question that was asked. So with that, again I advise that-- always read the problem in detail. Look at the units that you're working with and make the appropriate conversions because everything should be on your table of contents.