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3.091SC Introduction to Solid State Chemistry, Fall 2010 Transcript – Exam 1 Problem 5

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Hi I'm Sal. Today we're going to be doing problem number 5 of fall 2009, test 1. Make sure that you read the problem in full detail before attempting the problem. And there's also some things that you should know, pretty much background material. Before attempting the problem. And that's what I need, which is W I N. You will win if you know how to manipulate these equations.

The first equation is the energy of two charged species as a function of their internuclear separation. And the other equation is a function of just the separation between two ion pairs at equilibrium, which is given by r naught. And r naught is just simply the sum of the radii of the cation and the radii of the anion.

So if you look at this equation there's two components to it. The first component is actually the component that is responsible for the attraction of your charged species. And the second component is the repulsion of it. Because essentially ionic bonding happens because of your electrostatic interaction between an cation and an anion. So with this in mind we can go ahead and read the problem and solve it.

So the problem reads as follows. On the same graph below-- and this is the actual graph that we're going to be doing the problem on-- it says on the same graph below, for one, BeF2, so beryllium fluoride, and two, BeO, which is beryllium oxide, sketch the variation of potential energy with internuclear separation arc between a cation and an anion pair in each compound. The diagram need not to be drawn to scale however you must convey the relative magnitudes of key features.

So the first thing that I would do is write down my compounds that I'm using. So I'm focusing on beryllium fluoride, is the first one. So if I look at beryllium fluoride, I'm going to look at the relative magnitudes and charges when they're in their cation and anion state. So I know that for beryllium, beryllium forms a cation that is 2 plus. So it has a positive charge of 2, which means that it lost two electrons. So I can say that z plus for beryllium is plus 2 and for fluorine, when it's in the anion state, my charge is equal to minus 1. So 2 plus minus 1. So with this in mind, you can take this and it will help you solve the problem. Because like I said, the first part of the equation is pretty much the attraction part, which involves the product of your charges.

And I want to go ahead into the same thing for-- so this is for BeF2. And for BeO we have the oxygen 2 minus. So my anion has a z minus of minus 2 and my cation just has z plus of plus 2.

Now if you look at your equation over here. There's two things that will dominate at certain parameters. Now this value of n is known as the Born Exponent, and that has

a value between 6 and 12. So it's always greater than 1. And this is actually what's nominating your repulsion, so I'll do some colored chalk. So for the attraction part I'll circle it. And the fact that it's being attractive means that one of these charges has to be negative that will make the overall component negative. Right here because you'll have q1 times q2. And in our case if we look up beryllium fluoride, you have beryllium 2 plus you have fluorine minus, so if you make the product of those two you get minus 2.

And you have this other component, that is the repulsive part. So if I was to draw these independently, not as a sum, I know that for my attractive part, which is the negative, it should look something like so, as a function of r. And my repulsive should look something like so. And this makes sense because as your radius becomes smaller and smaller then essentially if you get below 1, your potential energy curve for your-- the component for your repulsion-- spikes up.

So if I was to superimpose these two, then I should expect that the curve to look something like so. Now this is good because this is exactly how the curve should look. And there's some characteristic features here that we want to go ahead and use BeF2 BeO2, draw on the same diagram to compare together. And this point right here on your r-axis is simply just your r naught. So it's just the sum of your cation radius and your anion radius. And this valley here is your energy at r naught. Which is the second equation that you should know how to apply.

So if I want to analyze my system, how do I know which one has a bigger radii than the other? Well I know that my cation is common. So in both cases I'm dealing with beryllium cations. But I'm dealing with a different anion. Now I know that both fluorine and oxygen anions have the same number of electrons, from looking at the Periodic Table of Elements, or their charges that they have. But fluorine has one more proton. So what that does is that it allows the fluorine to pull the electron cloud tighter together and that decreases your radius. So just by looking at the Periodic Table of Elements, I can already assume that my radius for my fluorine should be less than the radius of my O2 minus anion.

So if I look at my system than I know that if I want to look at the internuclear separation, the r naughts of the two compounds, then I should assume-- or have an educated guess based on my data that I have here-- that r naught for beryllium fluoride should be less than the r naught for beryllium oxide. So this allows you to put the position of your radius on your curve.

So I'm going to go ahead and just redraw the a new axis over here just to compare both of them so you won't confuse yourself. So we know this is the energy of our system. And we concluded that our, that the radius of your beryllium fluoride is less than the radius of beryllium oxide. So I can go ahead and mark this as r naught of BeF2 and I'll mark that as r naught of BeO.

So this tells me exactly where the low point of my potential curve should lie. But how do I know how deep it sits in the well? Well that's going to be dictated by the equation that governs the energy at r naught. And that's our simple equation of when it's the function of r naught. And if you look at the equation, the equation is just the product of your two charges. So if we come back and we look at our analysis here, we know that if I multiply these two charges together, you know the combination of these two, should be, q1 or q-- beryllium 2 plus, I'll call that q1 and

I'll call this one q2. The product of these two gives you minus 2. But for this one, q1 q2 gives us minus 4.

So this tells me that the electrostatic interaction for beryllium oxide is a lot stronger than beryllium fluoride. And it makes sense because you have plus 2 and minus 2 being attracted to each other instead of plus 2, minus 1. So on my graph I can assume, I can guess, that my value of my beryllium oxide should sit lower, more negative, on the potential curve than beryllium fluoride. So if I designate this as the low point for my beryllium fluoride then my curve for this system, for that particular compound should take a certain type of shape.

And so again, this is your energy, the bottom point of r naught. And if this is the energy given to the fact that we have a higher magnitude when you multiply the two charges together, then it should sit lower on the potential well. And this will be my low point. So my curve should also look something like so. So if you were able to do this on the exam you would have gotten full points, which is good. And, again the key points about this problem is just knowing what equations to use by reading the problem. The problem talked about internuclear separation, well we've learned in class how to treat those problems and how to use equations to be able to describe the way that the energy should look, which is a good visual. And by looking at the Periodic Table of Elements, just thinking about how many protons, how many electrons certain cations have, you should have an estimated guess of what your ionic radius should be. And with that you can go ahead and look at the math. Look where that parameter plays a role in your equation. And then decide whether or not it'll be greater or less or what have you. So with that in mind, I dare you to try the problem now and give it a good shot.

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