MIT OpenCourseWare <a href="http://ocw.mit.edu">http://ocw.mit.edu</a>

3.091SC Introduction to Solid State Chemistry, Fall 2010 Transcript – Exam 1 Problem 2

The following content is provided under a Creative Commons license. Your support will help MIT OpenCourseWare continue to offer high-quality educational resources for free. To make a donation or view additional materials from hundreds of MIT courses, visit MIT OpenCourseWare at ocw.mit.edu.

Hi, I'm Jocelyn, and we're going to go over Fall 2009, Exam 1, problem number 2.

So as with every problem, we want to first read the full question. In box notation, give the complete electron configuration of each of the following gas-phase species: calcium 2 minus and magnesium 4 plus.

So the first thing to note here, is you need to know what electronic configuration is. If you don't, you might want to go back and review that material, but it is basically assigning electrons to orbitals.

The next thing you need to know is what box notation is. And Professor Sadoway introduced that in class, and you'll see, as I go through this, a refresher of that, if you forgot.

So to assign electrons to orbitals, we first need to know how many electrons we have. So let's start with the first part of this problem, which is calcium 2 minus. We will look at our periodic table, and see that neutral calcium has 20 electrons. So calcium with no charge has 20 electrons. The 2 minus tells us that it has 2 extra electrons. Right? Because electrons have a negative charge. So we have a total of 22 electrons that we need to assign into orbitals.

In order to actually do the assigning, we need to follow the three rules that Professor Sadoway introduced in class. So I will put that over here.

The first rule is that you need to fill them, at least for a ground state species, in order of increasing energy. That is, you want to fill up the lowest energy orbitals first, and then move to the higher energy orbitals. This makes sense because ground state species want to have the lowest total energy possible. So the first is--

Now, how do we figure that out? Well, there's a few ways. One way is a nice trick that you can do on the side of your page or something. And it goes like this. So we have our s, p, d, and f orbitals. Right? We know that s can be in the first energy level up. We know that p starts at the second energy level, d starts at the third, and f starts at the fourth.

The tricky part is that you don't just fill up 1s, 2s, 2p, 3s, 3p, 3d. There's a little bit of mixing up of the energy levels versus the actual energy of the orbital.

So a nice side of the page trick is to draw diagonal lines down through these numbers. And if you follow these arrows, you'll fill up in order of increasing energy. For example, after you fill up the 2p, you're going to fill up the 3s then the 3p, the

4s, and then you'll go to the 3d. If that doesn't make sense, you might want to go and review a little bit about the orbitals in your textbook, or other resources.

The other way you can think about the ordering of the energy of the orbitals, is to be familiar with the periodic table. So we're just going to have an aside over here. And a general, very rough sketch of the periodic table would look something like this. OK? You have your alkali, alkali earth metals over here. You have aluminum, oxygen. Your halides, your noble gases over there.

But the way I drew it here is in what we call blocks. So this is your s block, and then we have our p block over here, d block, and the f block is down here.

So once you get more familiar with electron configurations, you can actually looks towards the periodic table, and know, depending upon where your element is in the periodic table, what its electron configuration is. Or at least the electron configuration of the valence electrons.

OK. So moving back to our trick, which we'll use now, we know that we have 22 electrons, and we know the order that we need to fill the orbitals. So let's start writing out our boxes, which is how Professor Sadoway wanted us to answer this problem. So we have 1s, our 2s, 2p. If you're unsure why I'm only drawing 1 orbital for s and 3 orbitals for p, again, you might want to go review that beginning orbital material. So we filled, we have 1s, 2s, 2p, 3s, then we're going to do the 3s here, we're going to do the 3p. And after the 3p, we do the 4s, and after the 4s, we do the 3d. Which has 5 boxes, right?

So now that we know which orbitals we're going to fill, we need to know some more rules about filling them. So the second rule, over here, is the Pauli exclusion principle, which says that no two electrons can have the same quantum numbers. For us, that means that we basically can only have two electrons per orbital, and of opposite spin. So that's something we need to remember for this.

The third is Hund's Rule. And that is, we want to have as many unpaired electrons as possible. So that will come into play when we're filling up our boxes in just a second.

If these are confusing, again, we want to look at the lecture material. So I forgot my boxes here. Now let's start the fun part of filling up the elections. So we fill up 1s, spin up and down, the 2s, spin up and down. So that's 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, and we have 2 more. So in the 3d, we're going to do 21, 22. And I separate them out because of Hund's rule. We want to maximize the number of unpaired spins. They both spin down, or both spin up, but they will be the same spin, and they will be in different orbitals.

So this was the answer for this part of the problem. Now let's move to the second part. And maybe you can try by yourself, and then we can do it here.

All right. Now we're going to do the second part of this first part of the problem number 2. So it asks us for the electron configuration in box notation of magnesium 4 plus.

So again, we're going to determine how many electrons we have. Which, neutral magnesium has 12 electrons. But the 4 plus signifies that we have 4 less electrons than neutrality, and so we subtract 4, and we have 8. With 8 electrons to work with,

we again want to write down our boxes using the energy level tricks that we have. And now we can fill them up.

The Pauli Exclusion Principle tells us 1 spin up and 1 spin down per orbital, and Hund's rule tells us that when we fill up this 3p, we're going to try to maximize the number of unpaired electrons, and then, when we have to, we pair up the spins.

So that's another main mistake that people make, is they pair up too many spins, violate the Pauli exclusion principle, putting 2 electrons of the same spin in one orbital, or something of that nature. So this again is the correct answer, and would-oh! I'm sorry. This is 2p. I'm sure you guys caught that. And would have awarded you full points in this part.

All right. Now we're going to start the second part of this problem, part B. So first we want to read what the question is asking. Give the chemical identities of the species with these ground state electron configurations.

So now we're working in the opposite direction. In part A, we were given a chemical species and asked for the electron configuration. Now we are given the electron configuration, and asked for the chemical species.

So the first one has the electron configuration of xenon. So this is a noble gas configuration, plus what turns out to be 27 electrons. One way you can do this, is to go to xenon, which is in the fifth row of the Periodic Table, and count through 27 electrons, remembering that when you get to the d on the sixth and seventh row, you need to go to the f block, which is signified in this problem by having f block electrons. Count through the f block, the d block, and end up at thallium.

Or if you are familiar with the Periodic Table enough that you can recognize the valence electrons are in 6p. And the 6p only has one electron in it. So that tells me, xenon is in row 5. This element is going to be in row 6. I go to the first column of the p block, which signifies that there's one electron in that 6p orbital, and I see that it's thallium.

That's the quicker way to do it. On an exam, you might want to be that familiar with the periodic table to be able to do that, because you're certainly time-crunched, a lot of times. So because that's a neutral atom, that method will work very easily. The second part is a little trickier, because it has a charged species. So we have a net charge of 4 plus, an electron configuration of argon and 3d5. This may seem a little confusing at first glance, because we always fill the 4s before the 3d. But when you're ionizing an atom, it turns out you take electrons from the 4s first, even though it's of lower energy. So that's a little subtlety that's not too important to this problem, but it may have tripped you up when you were looking at this, and certainly caused some problems for the people in this class.

Again, we go to the periodic table and we see where argon is, and then we go to the next row. The way I like to think about this, is this is the electron configuration, missing 4 electrons. To find the element that has this charge, I'm just going to add back in the electrons, go to that position in the periodic table, and that is my elemental species.

So we want argon plus, instead of 5 electrons-- I'm sorry, the problem says this is a 3-- instead plus 3 electrons, we are going to go to argon plus 7 electrons. And going

through the periodic table, you'll see that that leaves you with manganese. Adding the 4 plus, because that is part of this chemical identity, we get the answer of the problem.

So again, the charged species make this a little more complicated. The easiest way is to go back and add in the missing electrons, because that is your chemical species, and then remember to signify that there actually is that charge for your answer.

So moving on to part C, it asks us, write the quantum numbers of one of the 3d and one of the 4s electrons in iron. So this requires a knowledge of what quantum numbers are, and what values they can have.

So let's start with the 4s, because that's a little more straightforward. He tells us that we have an n quantum number, I quantum number, m and s. And, hopefully, we all know that n is the principal quantum number. It's basically your energy level. I gives you what type of orbital you're in. Right? If you're in the s, the p, the d. So it just tells you your orbital shape, basically. m gives you the angular identity of the orbital you're in. We didn't really talk about that in depth. We just need to know, it tells you which of the p orbitals you're in, or which of the d orbitals you're in. So I'll say, which orbital. And the s is your spin. Right?

So for a 4s electron, it doesn't actually matter what the identity of our species is. So that he tells us is iron is kind of extra information. A 4s electron already has 3 of its quantum numbers set. So we know that n equals 4, for s, I equals 0, and m, which orbital, s only has 1 orbital. So m always equals 0 for s, and your spin. And I'm going to make that a script, just so it's less confusing, is plus or minus 1/2.

So the answer to this problem could have been 4, 0, 0, 1/2, or 4, 0, 0, minus 1/2. Three of them are set by the fact that this is the 4s orbital. The spin can either be plus or minus 1/2.

If you're unsure of where I got these numbers, and why they have to be such, you may want to review the lecture on that.

So moving onto the 3d quantum numbers, we know that n is 3, I for d is 2, m is negative 2, negative 1, 0, 1, or 2, right? Because there's 5 different orbitals in a d set. And then again, s can be plus or minus 1/2.

So picking one set of those, you could have said 3, 2, minus 2, plus 1/2, or any combination of 3, 2, and the m and the s. You don't have to get the exact same answer as your neighbor or someone else you're-- well, you shouldn't be looking your neighbor's paper, or a classmate, but these do signify that you're in a 3d electron.

## MIT OpenCourseWare <a href="http://ocw.mit.edu">http://ocw.mit.edu</a>

3.091SC Introduction to Solid State Chemistry, Fall 2010

Please use the following citation format:

Donald Sadoway, 3.091SC Introduction to Solid State Chemistry, Fall 2010. (Massachusetts Institute of Technology: MIT OpenCourseWare). <a href="http://ocw.mit.edu">http://ocw.mit.edu</a> (accessed MM DD, YYYY). License: Creative Commons Attribution-Noncommercial-Share Alike.

Note: Please use the actual date you accessed this material in your citation.

For more information about citing these materials or our Terms of Use, visit: <a href="http://ocw.mit.edu/terms">http://ocw.mit.edu/terms</a>