

Computational Materials Physics (2024)

webinar 04 – crystallography

Welcome to the next feedback webinar which is now on crystallography as you will have noticed during the past week. Before going to the science let's look at how it goes with the project. So three teams have started I've seen and perhaps a fourth team is on its way that I still have to verify with these people. At least three work plans have been submitted and probably tomorrow the teams will get some feedback on these work plans. So the project seems to have started well. And that was the only housekeeping announcement so we can tackle the crystallography topic. And usually at this stage of the course and this was this year not different people have two different feelings with the crystallography module. And I've summarized these in these two quotes. Some people, the quote at the left-hand side, they find this a bit different from the DFT topic for instance of the past weeks and yeah not that scientific, not that deep. While others, the quote at the right-hand side, like it that after two weeks of mind-bending thoughts about DFT that this was something practical and hands-on. And the two opinions are right. It is a very different topic. But we need this topic to be able to handle the input that we will be giving to our DFT codes if you cannot properly visualize a unit cell and if you do not understand what are the items that you have to deal with. To provide to the DFT code in order to specify a given crystal, well then you would be working blindly. And therefore we started with what is actually the most important aspect of this week, the CIF file and the kind of information that is contained in the CIF file. And I showed you some repositories for obtaining CIF files, so a list of several resources that are not completely overlapping with or not completely identical to each other, they are to some extent overlapping, but if you need a specific crystal it makes sense to go searching in any of these resources. And in order to train ourselves in the use of CIF files, I gave you a chemical formula of a crystal that is on purpose very complex. So if I would give you the chemical formula for rock salt, then I don't doubt that many people could draw how the unit cell of rock salt looks like, but if I give you this chemical formula, then very likely nobody will be able to do that. So therefore, let's start from this chemical formula, search a picture of the unit cell, and download a CIF file for this unit cell on your computer. And then transform that CIF file into input for a DFT code, be it Quantum Espresso or any other DFT code that you would prefer to use. And it's not needed to run that calculation, because for such a unit cell that will very likely be a very time-consuming calculation. No, it's just to produce the input file, such that you gain confidence that whatever CIF file you can find, you can convert that into input for your code. And this is something that once you have gone through the basic calculation of two weeks ago, well if you repeat this step here, then you can immediately do that. So you go to a database, the COD database for instance, you download the CIF file of this crystal, which is this 901 and something more, and some more characters, and you apply the same comments with CIF2Cell that you also applied to the silicon example. So CIF2Cell, name of the downloaded CIF file, and then you go to the database, and you download the CIF file of this crystal, P and then QuantumEspresso to indicate that you want to produce an input file for QuantumEspresso, O, which gives you then the name of the input file, and we will call it neptunite.in, because neptunite is the general name of that complicated crystal that I showed on the previous slide. Now why do DFT codes, and this is a small side step, why do DFT codes, why do they, why don't they work directly with CIF files? Because I'm trying to sell to you the idea of a CIF file as the most common way, the most general way, to note how a unit cell looks like, to define how a unit cell looks like. Wouldn't it be easier that every DFT code just reads from these CIF files. And for historical reasons this is not the case. Different DFT codes usually read the input file, the input crystal structure in their own convention. The struct file for Win2k, the poscar file for VASP, the .cel file for Castep, and the .in file for Quantum Espresso. Now this means that if you have a calculation with one code, and you want to repeat that calculation with another DFT code, that you need to convert that crystal structure information. And if we consider only these four codes, that gives already the need for six different converters, if you go from the poscar in VASP to the .in file in Quantum Espresso, you need a converter. But from the poscar in VASP to the struct in

Win2k, you need another converter. And the more DFT codes you consider, the larger the number of converters you need. This is where CIF files kick in as being something useful, because every code has a converter, back and forth, to CIF formats. So if you can work with a CIF file, then you can convert it to a poscar file, or to a struct file, or to an .in file, and you only need as many converters as you have DFT codes. So therefore it's useful to be able to work with CIF files. Also because the results of experiments in crystallography, they are stored in databases in the CIF format. So if you do that with that Neptunite CIF file, the visual picture looks like this, and I guess most of you have found something like this. And we will use now this example and two other examples, to exercise, to train ourselves with crystallography. Not with the theory of crystallography, that is not what this module is about, but rather a kind of practical crystallography. Which elements of the theory of crystallography do we need in practice to do something with our CIF files? And therefore let's have a closer look at what is inside a CIF file, the one here for this Neptunite. The first thing you notice are three lines that basically tell the same. They tell, they give you information about the space group of that crystal. And they do this in different name conventions, by the number in the international tables of crystallography, by the Hall symbol, or by the Hermann Mauguin symbol. Three different ways to convey the same information. If you look at the Bilbao crystallographic server, one of the resources that was quoted, then you will find there, for instance, this list of the 232 space groups that are possible, and the one that we are interested in for Neptunite, space group number 9, is indeed present in this list. You see here two different entries, we will see later what that means. After the space group, the second important piece of information is everything you need to quantify the shape and the size of the unit cell. So not the atoms that are inside the unit cell, but the unit cell itself. And we have seen before, that there are six pieces of information, required for that. You can give the three lengths of the three edges of the unit cell, and the angles between these three edges. So six pieces of information. Or alternatively, if you specify these as vectors, the three vectors A, B and C, but they have some relations with respect to each other, so these are not nine independent degrees of freedom, and there will also there be six degrees of freedom. But the most common way is to use the length of these three vectors, and the angles they make with respect to each other. So these are the six numbers that are listed there. And then comes a list of coordinates for the different atoms in the unit cell. So we have now defined the box in which these atoms can be, a box with some volume and some shape, given by these six parameters, and now we populate that box by atoms. And we give always the name of the element, and the three coordinates of the position of that element. On top of that we also have symmetry operations, because there is some symmetry present in that unit cell, very often, and therefore it is not required to give every coordinate of every atom in the unit cell. No, you can give the coordinates of one representative atom, and then the list of symmetry operations that is allowed here, and that will copy that atom to different other positions in the unit cell. So that is how you see this in the CIF file. If you look on the other hand at the input file for QuantumEspresso, there you will see the same information, but encoded in a different way. The shape and size of the unit cell, rather than specifying this by these six numbers, you will give the components of the lattice vector. So the lattice vector A, the first row of this matrix in the cell parameters block, these are the three components of that lattice vector. Now, when you translated the CIF file from the database to the input file for QuantumEspresso, some of you have run into an error message. You see one possibility of that error message here on the screen. And some people noticed and wrote that in the forum, that if you use a particular CIF file for Neptunite, you run into problems, but if you use another CIF file for Neptunite, then that problem is not there. This has a reason. Here is another screenshot. If I reproduce this in my installation of VirtualBox, then of course I get the same problem. And why is that? Well, if we look into a CIF file that does not work, that gives this error, then I see something like this. If I do this for a CIF file that does work, then I see input like here on the bottom. And what is the difference? Well, in the one on top, the one that doesn't work, you see the name of the element, followed by a number, and in a few cases, also followed by a character. Silicon A, Silicon 2A. That does not happen in the second case. And it's that what is causing the problem here. That converter

CIF2Cell, assumes that the first string in such a line of coordinates, gives you the name of the element, and at most a number. Nothing else. Not a letter from the alphabet. So if you would take that first CIF file, and you replace all the characters by numbers, or you would just erase them, and give only the name of the element, that's also OK, then you will have a CIF file that can be converted without problems. And the interesting thing is, for the people who have run into this problem, you could have found the discussion with the solution of this, already on the forum. In the forum, some time ago, somebody raised this question, and there is a whole bunch of answers, that eventually leads to the solution. So I hope that by leaving these forums there, that if the need arises, you can solve some of your problems by browsing through the forums. Another question that was sometimes raised on the forum is, and sometimes you have these kind of warnings, site occupancies not found, assuming all occupancies being one. What does that mean? First of all, that's an innocent message. And what does it mean? Well, you can specify in a CIF file, for each of these coordinates, what is the percentage of these positions that are actually occupied by atoms. In an experiment, a CIF file that is a result of a crystallographic experiment, X-ray diffraction for instance, on a material, it could happen that you conclude this position is occupied by iron atoms, but 80% of these positions are empty, they contain a vacancy. Or, 80% of this position is occupied by iron, and 20% is occupied by silicon. This is a disordered site. So, for that reason, you can specify in a CIF file, next to the coordinate, what is the percentage of that coordinate that is occupied by the element that is at the beginning of the line. That makes sense for an experiment, but that does not make sense for a simulation. Because when we build a unit cell, that we will give to DFT, we need to put either an atom on a site, or nothing on a site. We can't put 80% of an atom at a site, or we can't put a mixture of two atoms at a site. So therefore, in a CIF file that is used for DFT input, the occupancy, so what is the fraction of the sites that is actually occupied by the element, is always 1. And therefore it is not mandatory to write the occupancy. And CIF2Cell, when it reads a file that does not have occupancies, will say, I didn't find any, so I will assume they are all 1. And if that is what you wanted, then this is perfectly ok. Then another question on the forum, that is a trigger to think a bit more deeply about the CIF file. Somebody noticed, if I make that input file for QuantumEspresso, I seem to have two formula units. Is that correct? And how did this person come to this conclusion? If you count the number of atoms that are in the chemical formula in the beginning of the CIF file, so I have here all the atoms that appear, then you have 40 atoms. And if you look in QuantumEspresso, in the input file that we created, there appears to be not, which is the key word for the number of atoms in the unit cell, 80, so twice as much. Is that correct? We want to make a unit cell for a chemical formula with 40 atoms, and we have one with 80. Yes, that is correct, because a unit cell can contain more than one formula unit. Even a primitive unit cell that cannot be further reduced can contain more than one formula unit. So we have to distinguish the concept formula unit from the concept unit cell. They are two different things. Ok, let's move to the chat to see whether something is being asked. Not right now. So we continue with the second exercise that will give us some experience about the use of CIF files. And that is an exercise where you start from one word. I gave you the word letharge. Only that, and then all questions that come can be answered starting from that word. So letharge is the name of a crystal, and I ask you to Google for its chemical formula, and then search for that crystal in the COD database or in any other database. And some further questions that I will not read right now, what is the space group, and so on. So Google for its chemical formula, you get results like this, letharge, and you read there in one of these links that goes to Wikipedia, letharge is a lead oxide with chemical formula PbO. You even read in Wikipedia what is the space group, that is one of the questions that will follow, so you have already that information too. So letharge is PbO. Then we have to search for that crystal in the COD database. And if we search for everything that has lead and oxygen elements and nothing more, you get a list where for some cases we have PbO. So the right relative ratio, one to one, so that could be our letharge crystal. There is a bit more to that, we will come to this in a few minutes. Now somebody asked, if you do this, then you see in the COD database that there are often multiple CIF files for the same crystal. I search for PbO and I get here already four crystals. So what could that be? Well, sometimes different, of the same

chemical formula, PbO, can appear in different crystal shapes. I have here PbO, that is in this space group, P4NMM, but two lines deeper, I also have PbO, same chemical formula, in space group PbCM. So two different space groups, two different crystal structures for the same chemical formula. That's perfectly allowed. Or, sometimes, COD is a mainly experiment-oriented database, you will have experimental data for the same crystal, the same chemical formula, but old and new experiments, experiments from sometimes even 100 years ago, and experiments from last year. So then it's up to the user to take the experiment that is most precise, or most reliable. And often that will be the most recent experiment, not always though. And a second reason, and that is illustrated by the first and the last line of this table, you can have the same crystal in two different crystallograms, in two different graphic settings. And we will come to that in a few minutes. Good. We had to answer the question what's the space group of lethargy? And I already told you, in Wikipedia you can see this, and in the COD database, the screenshot you just had, we also have this same P4 over NMM. So that's the space group. And if we look in the Bilbao crystallographic server, which number is this? P4 over NMM? It's number 129. So this is a unique tabulation. If you find that symmetry symbol with a given number, that will always be the number of that space group. What are then, the Wyckoff positions for all the atoms in that unit cell? How can you find that information? The most straightforward way is to go to the Bilbao crystallographic server, to take the WigPOS program, and then you will be confronted with this window, where you can put the number of the space group, so 129, and then you have to click one of these three buttons, that are for many people confusing. What should you take? Well, here the practical thing to know is, there are indeed, for many space groups, multiple ways how you construct that space group. It has to do with, where do I take the origin, how do I take the orientation of the lattice vectors? There are many equivalent possibilities. All these possibilities, they are listed in, or not all, many common possibilities are listed in the International Tables for Crystallography, volume A, that was once a book, now this is more a web resource, where basic crystallographic information is constructed and reported. So the ITA settings are a set of possibilities to construct a space group. And one of them is recommended as the default. And that means, if you don't have any reason not to do that, then please report a crystal in that space group, report it in that setting. So if you take the left hand side, button here, you will have the recommended representation of that space group. If you want another of the equivalent settings, you can first press the right button. If you want a setting that is even not contained in the ITA settings, there can be reasons why you want to examine a crystal in a very non-conventional setting, then you can define the setting you want in the middle button. But if you take the default setting, you get a table like this. Where I then ask you find here the lines that correspond to the lethargic crystal. Which is not obvious for everybody how to do it, so we will do this further step by step. And that is most easily done if we start from a picture of that lethargic unit cell. And then look at the coordinates of all the different atoms. I can find the picture on the crystallography open database. This is the entry for lethargy. You see usually this type of pictures as default. But if you right click on this graphical window, and then you take from the menu, you get symmetry. And then you take this second last line. It is here in a Dutch version, but you can have it in English or in many other languages. So if you take these lines, then you will get your unit cell in a view where all the positions in the unit cell are occupied. Not as in the previous slide, where you have a minimalistic view, where only one representative position per Wyckoff site is occupied. No, all the positions in the cell that can be occupied are drawn here. That is the most intuitive picture to look at the unit cell. In Vesta, another visualization tool that you can use for free, this would look like this. And in this example here, so that is the same picture as here, but Vesta can also draw the atoms that are just outside the unit cell. That is sometimes useful to have a better view on how the atoms are actually coordinated. Now in this view on Vesta, I can read the coordinates of the atoms. For instance, this lower left lead atom has coordinates 1 quarter, 1 quarter, 0.23. And the upper right here has as positions 0.75, 0.75, 0.77. If I now go to this list of Wyckoff positions, then I find indeed a line that has 1 quarter, 1 quarter and some number. And 3 quarters, 3 quarters and the opposite of that number. And if you then know that the opposite is identical to the one complement, so if this would be 0.23, if Z would be 0.23, then

minus Z is minus 0.23. But minus 0.23, that means I go under the floor of this unit cell to the negative range, and that's the same as entering from above. So this position here would be at minus 0.23, but also at 1 minus 0.23, which is 0.77. So from this, we can indeed conclude that Wyckoff position 2C is the position of the lead atoms. And here was a question, not of this year, but a question of previous years that gives some insight. If we want to build such a unit cell, if we want to populate that unit cell ourselves, what does it mean that we have an undefined number Z here for the line below, for the 2B position? We have a full coordinate, we can put the atom there, but here we have a Z. What does that mean? Well, I will elaborate on that example later on, but it basically means that for symmetry reasons, there is no value for Z that is anyhow special. Whatever value for Z you take, you have a position that is valid within this space group. Nature will have chosen a value for Z, so your lethargic crystal there, Z is 0.23, and not 0.47 for instance. So nature has chosen a solution, but symmetry does not dictate what that solution should be. Then, again reported in the forum, some people say, good, I have taken my CIF file from COD, and I tried to find the Wyckoff positions, but it doesn't correspond to that 2C position. I see something totally different. Why is that? And that is related to the fact that we have in the COD database this space group with a 1 and a 2, and these mean 2 different settings. So COD reports the same chemical formula in the same space group, but with 2 different settings. And if you take the other setting than the one we were using before, then you will not have the same Wyckoff positions. Let's illustrate that. If you would click the button with ITA settings, then you will see for this space group 129 that there are 2 of them. One with origin choice 1, and one with origin choice 2. And these are the 1 and the 2 that you saw in COD. And if you inspect further what are their properties, you will get here transformation matrices, where you have a rotation and a translation, and where you can convert origin choice 1 into origin choice 2, or the other way around with the inverse of this operation. Here they are listed next to each other. In the standard setting, which was the one we were looking at, 1 quarter, 1 quarter z, that's a 2c position, but that same 2c position has in the other setting has as coordinates one half, zero z. It looks quite different, but it is exactly the same position only in a different setting. And we can draw this. The thing we have been looking at so far, that was origin choice 2, with 1 quarter, 1 quarter z, origin choice 1, here the unit cell looks like this, the lead atom is in the left face, and therefore, due to periodic boundary conditions, you draw it a second time in the right face. This lead atom is in the front face, and its periodic image is in the face at the back. Why are these two settings relevant? Why do we prefer one over the other? Because origin choice 2 is the default setting. Well, in origin choice 2 we have a few interesting features. I draw here this green plane, and let's now look in the plane of that green surface here. So, this would be that green surface, and there are two lead atoms in that plane. So, this and this lead atom, these are these and these lead atoms. In origin choice 2, the origin of my axis system is taken here at the corner of the unit cell. And if I would now take the inversion of the lead atom here to the other unit cell, then there would indeed be another lead atom here. If I would put multiple copies of this unit cell, properly translated, if I go through the origin into the next cell in that green plane, then I will end up at another lead atom. So, there is inversion symmetry about the origin. If I would take the origin at a different place, namely at this position here, at an oxygen atom, if we now take this green square, which is now the left face of this unit cell, that would be this one, there is only one lead atom there. If I go through the origin to the next cell, there will be nothing there. So in origin choice 1, although it is a perfectly valid origin choice, you do not have inversion symmetry about the origin. And sometimes, having inversion symmetry can be useful. Some things are quite a bit easier with inversion symmetry than without. So if you have an origin choice that gives you inversion symmetry about that origin, then that is usually recommended to take that one. So this is why in this case, origin choice 2 is the default setting. And we have here a further comparison. So you have again the two settings and I have the two coordinates added here. And you can convince yourself that indeed the lead atoms have exactly these corresponding coordinates. Now, this gives not the position of every atom. We have two lead atoms in the unit cell and we have two of these coordinates. But in the CIF file you will see that there is only one coordinate listed. The CIF file for Letharge will have, say, 0.25, 0.25, 0.237 here and not the other lead atom. Where is that

information then? That is due to these symmetry operations. So the block of symmetry operations for Letharge, there will be 16 of them and if you apply all these 16 operations on that single lead coordinate then you will see that 8 of these 16 symmetry operations will bring the lead coordinate onto itself or on a periodic copy of itself whereas the 8 other ones will bring it on this other position in the unit cell. So effectively, by this single coordinate line and these 16 symmetry operations we find two atoms. If you do that with the lead atom in the other setting then the symmetry operations can look a bit different but the result will be the same you will have the two inequivalent sites. Ok, let me look at the chat ... nothing there so we continue one of the goals of this module is that you have some meaningful information that you can make sense of the concepts space group, unit cell and Wyckoff position and if I would summarize this then I would come to this relationship the space group, that is a kind of symmetry idea of your crystal and if you know the space group then the size and the shape of the unit cell the box in which the atoms are that is partially constrained if I give you a space group that is essentially cubic you will never find a hexagonal box so the space group constrains how the box looks like it doesn't define the entire crystal otherwise there would only be 232 different crystals possible but it constrains part of the box it also constrains the Wyckoff positions some of the positions in the box are allowed for atoms others not that doesn't mean there has to be an atom at that site but if the crystal has this space group then at least only at those sites only at those Wyckoff positions there can be atoms so the space group also partially constrains the atom positions the relation is different the other way around once you know the unit cell, the box and once you know the Wyckoff positions then you can uniquely determine the space group so it's deterministic in this direction not in the other direction and if I ask you give a full specification of a crystal for instance because you are expected to report a crystal you have found to a colleague who wants to do a calculation on this so that colleague asks you how does that crystal look like what will you then give as information, well you will give the space group plus all the degrees of freedom that are not constrained by the space group so if you have a cubic space group then you will only need to specify the length of one lattice vector, because the box is cubic anyway so if you know the length of one edge then everything is known if the space group on the other hand is one that is tetragonal then you will need two pieces of information to describe the shape and the size of the unit cell so all degrees of freedom that are not constrained by the space group should be reported for the unit cell and also for the Wyckoff positions in the case of lethargy, if we had an atom at this one quarter one quarter z position then you have to tell my lead atoms are at Wyckoff position 2c and the z coordinate has this value because that is a degree of freedom that was not fixed by the symmetry a few years ago somebody asked explicitly I don't see it how in the case of lethargy for instance, that z coordinate is not fixed by symmetry well, let's focus on that and let's try to demonstrate how this is the case so I take again my unit cell in origin choice 2 I have a lead atom at one quarter one quarter z you can see this with this axis system a is the x direction so one quarter in the x direction one quarter in the y direction and 0.23 into the z direction that's how I end up at this lead atom and I have drawn a green line through this lead atom and that is a rotation axis, a four fold rotation axis one of the symmetry elements of this position is a four fold rotation axis you can see that if you look from top down on this crystal so here you have the same unit cell but now from above and I take for instance this atom here here I will consider my four fold rotation axis well you can see there is here this square of oxygen atoms and another square of lead atoms so if I take a 90 degrees rotation about this axis that comes out of your screen then you will map the crystal into itself so that's a perfect four fold rotation axis if I would now change that z coordinate if I would move that atom up or down and that other atom correspondingly down or up because it has to be the complement then this symmetry will not change if these four atoms here which are on the same height on the same z value come up or go down the four fold symmetry remains intact if however I would change something to these one quarter one quarter which should be determined by symmetry so let's say this neighbor here I will not put it at one quarter one quarter I will put it slightly away from it then the periodic copies would also slightly move and my lead atoms would now be at the blue positions but if I go back to my four fold rotation axis this is now not a four fold rotation axis

anymore because it's not in the center of the square of the blue atoms so by changing a coordinate that was already dictated by symmetry you break the symmetry you can only modify the coordinates and if you do that in the proper way symmetry is not broken so that's the meaning that's the difference between a coordinate that is a free coordinate and one that is not another illustration for the same point now we look at that unit cell from the side and I see my two lead atoms at one quarter one quarter z two quarters minus z if I would change the z value then this atom would for instance go up and this atom would come down I have inversion symmetry about the origin for these two atoms if I take if I let this atom come down and this atom goes up I keep that same inversion symmetry whatever z value I take if however I would only change this z value so the minus z here would become z prime and I don't change this z value so if I would not obey the symmetry relation between z and minus z this atom comes down and now there is no inversion symmetry anymore with this atom so breaking the symmetry relations that are prescribed by the Wyckoff positions that removes symmetry elements from your unit cell and set the other way around the Wyckoff positions they are specified to such an extent that you can only modify the position properties that do not break the symmetry I go again to the chat still no question then we move on with another exercise still based on the Cypher where you will now try to build the CIF file for this crystal manually so you don't take it from a database no rather you read a description of this crystal and by this description that you find in a paper you build the CIF file yourself so how can we do that and I gave you for this purpose a template of a CIF file for P1 symmetry so space group number 1 which means a unit cell that has totally no symmetry and well by putting all the information that you know in that template you can start building your structure file and what many people do is something like this and I give the example here for origin choice 1 they look at the picture and they say ok I have an oxygen atom at 0 0 0 then I have another oxygen atom at 1 0 0 so you go 1 along the x-axis and then nothing anymore 0 0 there is another oxygen atom here and you have already 8 positions for oxygen and you do this until you have all positions inside the unit cell described but if you then give this to that Stokes program, FindSim where it will determine what are the symmetry operations for that crystal then you will run into errors and what is the reason for that you should only give one position coordinate for positions that are connected by periodic boundary conditions so what is the reason if we put an atom here at 0 0 0 what is the reason why we find it at all other corners of the unit cell that's periodic boundary conditions so we know this already if we know coordinate 0 0 0 we know that there will be atoms on all the corners so we need to specify that give it only once and then these errors will not appear so this would be an example of such a p1 sieve file where we have the a, b and c lattice parameter that gives a tetragonal box it's really tetragonal all the angles are 90 degrees we have just the identity symmetry operation the trivial one and I have two oxygen positions this one and this one not the periodic copies this one and this one and not the ones who are outside the unit cell because of course we have only to specify positions inside the unit cell and two lead positions where the z coordinates are each other's complement so this I can read from the picture this sieve file I can give to that stokes findsim program and if you do that it will give you in return this structure file where it tells you you don't have space group p1 this crystal has space group 129 it has recognized that for you and the only positions that you need to specify are these two and even there is a degree of freedom in the z coordinate of the 2c position it gives you already the Wyckoff letters 2c for lead 2a for oxygen so in situations where this is possible where your crystal structure is sufficiently simple such that you can visually read a picture you can transform this in this way from a sieve file to a sieve file that has complete space group and symmetry information and if you want to exercise more about that I have here one other example that is also sufficiently easy so I give you a drawing of a crystal with chemical formula YFS and that's really a chemical formula although it doesn't look like that that's yttrium and you see the positions of these atoms on the picture I have specified a few aspects of their coordinates you have the a, b and c of the lattice parameter so you could take this as an exercise put all this information in the p1 structure file run it through findsim and find a sieve file with all symmetry information included that's it for the discussions on the tasks of last week let me look once more at the chat nothing so what will happen next week

now we will answer the question if I get a sieve file save from an experiment or manually made and I wonder what would DFT predict about this sieve file what would be the lattice parameter according to DFT what would be the position of that atom according to DFT can we find that can we ask DFT predict me the optimal structure of the crystal in this sieve file that is indeed a question DFT can answer in the next two weeks in learning how this can be done so that's the important topic of geometry optimization there are practical exercises about this you will not be surprised and another practical aspect for those people who would follow these webinars live from other time zones keep in mind that this weekend in Europe to the winter time and that therefore the live moment of this feedback webinar in your time zone may be different if you don't make the same switch at the same time so therefore the times on the website are given in UTC so according to UTC it will be a one hour difference for the local people in the central European time zone nothing will change good so as you are expecting by now so now you will have five minutes to formulate your summary of the past week and to suggest an exam question and when these five minutes are done I will look for a last time to the chat if there are questions left there ok thanks for your contributions and then I go to the chat and I see nothing there and based on the experience of the previous weeks that means that probably nothing will appear so we can say goodbye here and I will see you next week with more reports about the geometry optimization bye bye