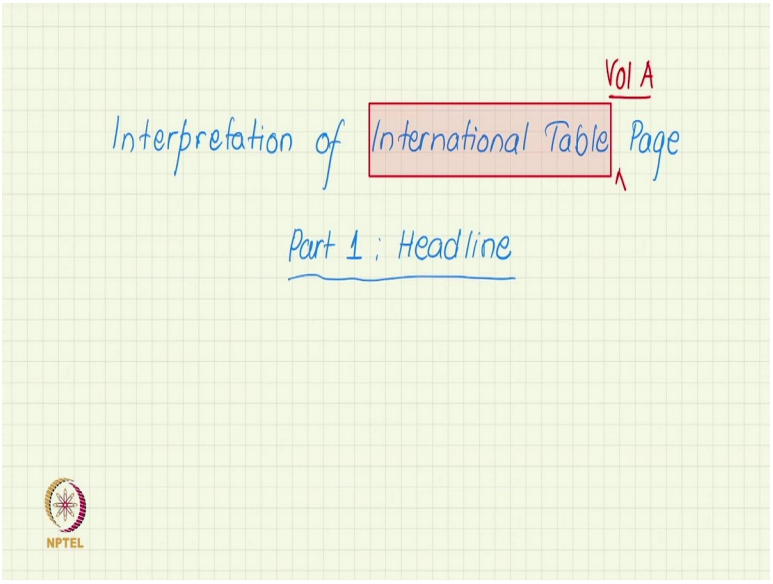
Professor 3D Space Groups VIII:
Interpretation of International Table Page
Part-1: Headline
Prof. Rajesh Prasad
Department of Materials Science and Engineering
Indian Institute of Technology, Delhi
Lecture 24 a

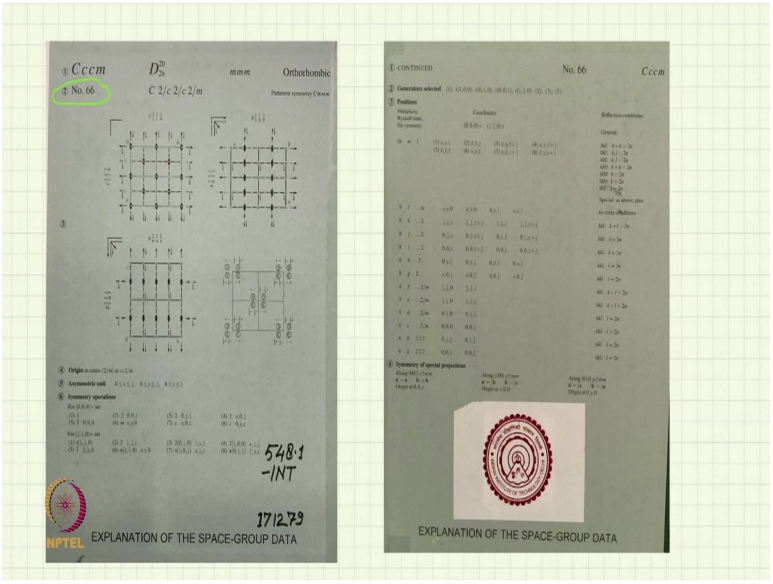
Hello, we have seen in the introduction to space group that one of the most important books for space group is the International Table.

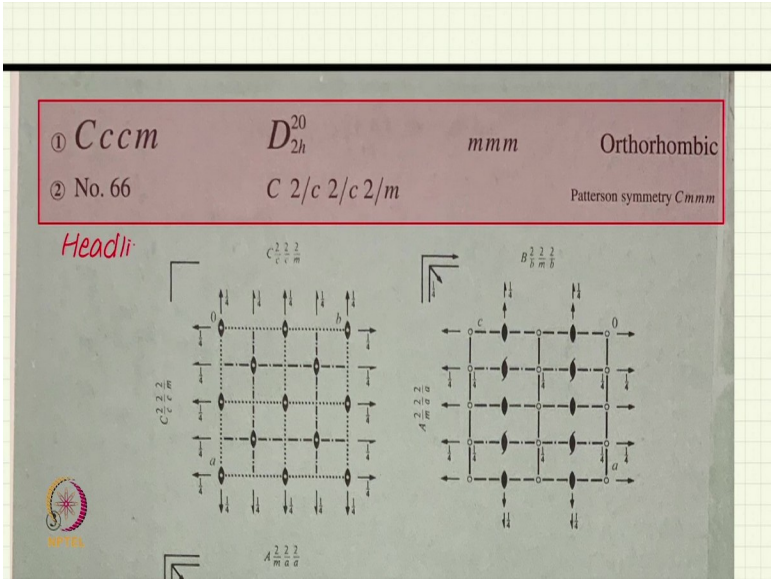
(Refer Slide Time: 0:21)

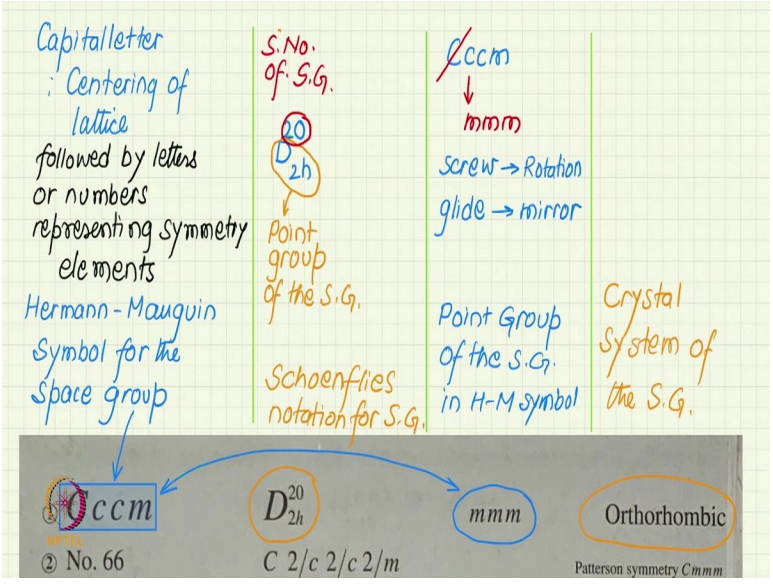


Actually, International Table has many volumes, and what we are talking about is International Table volume A. And there are pages in this book, which are devoted to particular space groups and all the details of that particular space group are given in the pages for that space group. So, we will look at the page we have already seen a view of the page when we gave the introduction to this space group. Now, we will see one of the page again and we will try to look at the details in the page one by one. The first part of the detail is what is called the headline.

(Refer Slide Time: 1:11)







So, let us see that. So, this is the space group page for a particular 2 pages devoted to a particular space group. So, let me look at the first page in a little bit of higher magnification and what you see in the top here, this particular information is what is called the headline? This is the headline. So, let us look at the headline in more detail. The first piece of information in the headline is here, which is written here Cccm. So, this is called the Hermann Mauguin notation symbol for the space group.

Let me put it close to the symbol itself I bring it here. So, this is the Hermann Mauguin symbol for this particular is space group. Now, this symbol consists of a capital letter, first part is capital letter which gives the centering of the lattice which means here capital C means the lattice is C centered. The capital letter is followed by letters or numbers representing symmetry elements. The symbol next to this edge also the space group symbol but that is in Schoenflies notation. So, this is Schoenflies notation or Schoenflies symbol for the space group.

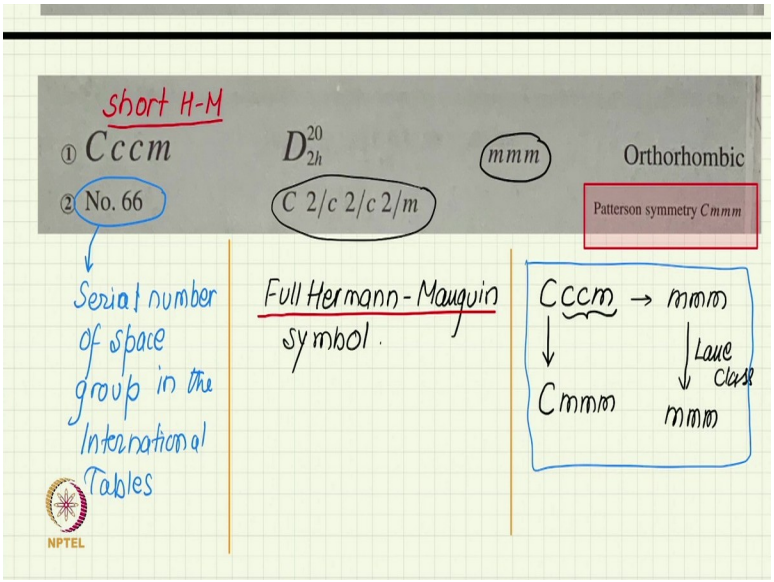
In their notation, if you look at this D 2 h 20. That D 2 h part just give the point group, point group of the space group and the 20 superscript 20 is just the serial number, the serial number of a space group. Which means that this is a space group 20th is the space group having the point group D 2 h from our point group video you know that D 2 h is a particular point group in Schoenflies notation. So, D 2 h 20 is the 20th space group having the point group symmetry D 2 h. Then we come to this third symbol mmm. This gives the point group of the space group in the Hermann Mauguin notation, this space group in Hermann Mauguin symbol.

So, mmm is the point group of this particular space group, these 2 are actually related and the relationship is very simple point group in Hermann Mauguin notation and the space group in Hermann Mauguin notation are connected to find the point group. Suppose, we have this point group Cccm all you have to do is to cross out the first alphabet the centering symbol and convert a screw axes to the corresponding rotation axis and a glide plane to the corresponding mirror plane.

So, here since cc are representing glide planes, so, they become mirrors and m of course, is a mirror. So, you can see that the point group becomes m m m. So, the conversion is screw to rotation and glide to mirror here there are no screw. So, we have not used a screw to rotation conversion, but we have used glide to mirror conversion. And finally, this last symbol here gives you the Crystal system of the space group. So, from the first line you know that this

space group belongs to the orthorhombic crystal system has the point group mmm has Hermann Mauguin symbol capital C followed by ccm and has Schoenflies notation D sub 2 h and superscript 20.

(Refer Slide Time: 8:18)



Now, let us look at the lower line of the headline. Here you will have just a number this number your serial number space group in the international tables. So, by seeing a space group 66 you mean this particular space group which is being discussed here and the next symbol is what is called a Full Hermann Mauguin notation. So, this is also the space group symbol just like capital C ccm we saw here only difference is that this is supposed to be a short symbol, Short H-M notation and this is supposed to be the Full HM notation.

So, here you have more details you can see. So, there you only know that there are glide planes c c and a mirror plane m here you are knowing that the glide planes and mirror planes all are perpendicular to the corresponding 2-fold axis. We will go into those details in a subsequent video. The final symbol Patterson symmetry we will not get into a lot of details of this.

But we will just tell you how to get the Patterson symmetry? For Patterson symmetry, all you have to do suppose Cccm. So, what you have to do is to keep the first centering letter, so that is C. And remember that the ccm was converted to the point group mmm point for that point group, if you remember in from our point group video, one of the videos were on larvae classes. So, you have to just write the larvae class of the corresponding point group.

So, in this case, the point group is mmm and larvae class also happens to be in this case, mmm. So, we simply write C m m m for Patterson symmetry, the significance of Patterson symmetry is in the analysis of diffraction patterns. We will not go into the details; we just note this sort of algorithm of how to convert the space group symbol into a Patterson symmetry symbol. We will not discuss it any further. Thank you very much.