Chemical Crystallography
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Lecture - 62
Origin of/Introduction to Systematic absences

CCT detector when you collect some 20, 30 images; we get about 100 to 200 reflections.

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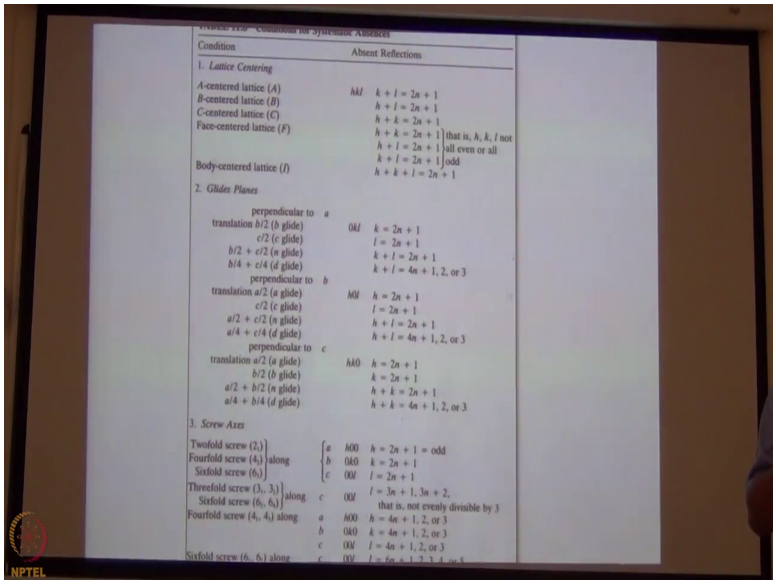

And out of those 200 reflections when you about 100 reflections, we have h k l general values and then immediately you have software to look for any systematical absences at of reflections from those h k l set. So, then you need able to predict whether it is a face centered lattice or a C centered lattice or something else. So, at the beginning if you only know whether it is

Student: (Refer Time: 00:51).

A centered lattice or beam team lattice based on that we collected data. At the end of data, we extend the data in terms of h k l versus intensity a big excel type of file. The formula that I have given today sometime ago gives you the total number of possible reflections and with today's diffraction software and sorry today's detector.

You collect same reflection multiple times with different orientation of the crystal. So, the h k l file that you will get where have 20, 30000 lines.

Student: (Refer Time: 01:36).

Maybe 30000 reflections of beam collected, some of them are repeated; some are unique.

Student: (Refer Time: 01:43).

It is not possible for anybody to physically look for those systematic absences among those some 30000 reflections. So, we again use the computer program to scan it be h k l set and tabulate them. Is there any set of reflections which are systematically absent in the entire list of 30000 reflection?

Student: (Refer Time: 02:08).

That then helps us to determine the space group of the crystal. So, this is an absolutely important. Now if your data quality is bad and some reflections which are actually going to be present, but you took some reason it is absent or it is having very very low intensity and it assume that it is absent. Then this space group determination is going to be wrong and if this space group determination is wrong.

Student: (Refer Time: 02:42).

We will not be able to solve the structure because you are trying to solve the structure based on a given space group. Of course, very recently a new version of selectors come. We solve the structure assuming everything as p 1, No matter what you needs l e if weak manner it is orthorhombic, tetragonal, primitive, or (Refer Time: 03:08) triclinic, or whatever. It assumes initially beta as p 1.

Student: (Refer Time: 03:13).

Solves the structure, and then applies this space group belonging to that point group that that is the point group which I have taken at the beginning, and then gives you best choice of space group entered. But above 1 year above it was free determined space group and then you plate it first structure solution. So, with this we will stop oh ok.

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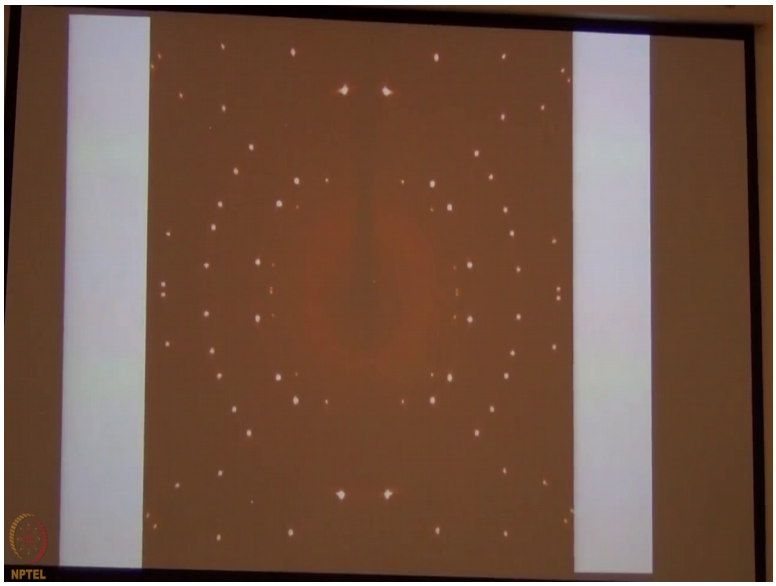

I wanted show you this oh sorry. So, what is this?

Student: With the system.

This is the rotation photograph as I promise to look you to show I told I show you because rotation photograph of sodium chloride crystal. See this dark region is the shadow of the big stock, and this is a square detector..

So, the direct beam is block, and these are spots that we have got by rotating the crystal in front of the x ray beam in 1 minute, this is to give you rotate one of the crystal. So, the crystal was mounted and it is rotated above this axis 360 degree in 1 minute.

Student: (Refer Time: 04:49).

What is happening? I do not know each axis is perpendicular to the beam; some axis is namely perpendicular to the beam. But of course, some reciprocal lattice plane, easier the plane of the beam and I am measuring it somewhere here.

So, when I am rotating the reciprocal lattice plane is rotated at some point or the other. Some reciprocal lattice point is crossing your (Refer Time: 05:24) and giving you diffractions for. Now you see it is totally centers matrix, you can see all the symmetries data are present in 1970. You see mirrors, you to see protocol axis and although. So,

every set of spot is symmetrical on the other side. This is a real rate protozoon photograph to see this symmetry is present in the data set.

So, if you take a rotation photograph of a crystal line material you will get from thing like that. For a triclinic system you pay at a large number of spots.

Student: (Refer Time: 06:11).

For cubic f, sodium chloride is fcc, you will get less number of spots like this. But always whatever you create is going to be symmetric, it will be center symmetric. In case of triclinic you will only see centre of inverse right. So, we will stop at this.