
Subject: Re: XDR format files

Posted by [Helder Marchetto](#) on Mon, 22 Oct 2012 09:19:58 GMT

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On Monday, October 22, 2012 10:50:09 AM UTC+2, sid wrote:

> Hi all,
>
> Please let me know how to open a xdr format file.
>
> I dont know the data type and size of the file. So I couldnt use the READU command.
>
> Please do help out in this regard.
>
> thanking you in advance.
>
> sid

Hi,

as far as I could see, xrd file are ascii files for x-ray diffraction with a header and the last line contains the "0 0 0" reflection.

Then you have at least two options:

1) you loop until you find the end line or the end of the file. The header lines start with a "[" and the data lines are composed of four numbers: hkl (Miller indices) and intensity. After you define the Line variable as a string (line="), you may read each line with the command:

readf, Lun, Line

Then check for the "[" character. If present, then it's header, otherwise not.

2) The other option is to count the number of header lines and the number of lines in the file by using the FILE_LINES(FileName) function. Then you can create an array or structure with the correct dimensions. Something like:

Reflex = REPLICATE({h:0,k:0,l:0,Intensity:0.0},FILE_LINES(XRD_FileName)-nHeaderLines-1)

And then you fill in the values.

Once you read a line, you can use the STRSPLIT(Line, /EXTRACT) function to get an array of four elements where the first three are Miller indices and the fourth is an intensity.

I hope this helps.

Cheers,
Helder
