Subject: Re: XDR format files
Posted by Helder Marchetto on Wed, 24 Oct 2012 08:39:55 GMT
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On Tuesday, October 23, 2012 11:29:37 AM UTC+2, sid wrote:
> On Monday, October 22, 2012 2:49:58 PM UTC+5:30, Helder wrote:
>
>> On Monday, October 22, 2012 10:50:09 AM UTC+2, sid wrote:
>>
>
>>> Hi all,
>
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>>>
>>
>
        Please let me know how to open a xdr format file.
>>>
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>>
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>>>
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>>
>>> I dont know the data type and size of the file. So I couldnt use the READU command.
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>>>
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>
>>> Please do help out in this regard.
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>>>
>
>>
>
>>> 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 cound 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_FileNam
e)-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
>
>
  Hello sir,
        The file which I am having is XDR(external data representation) files. Please let me know
how to open this kid of file.
> thank you
>
> sid
```

Ups, I got that one completely wrong... My browser auto-corrects the inputs depending on my

usual research field queries! Anyway, if you want to switch to xrd files, they seem easier to read :-)
Cheers, h
h