

[RMCPProfile-users] R: Re: R: Re: get_gsas_bragg

[helen.playford at stfc.ac.uk](mailto:helen.playford@stfc.ac.uk) [helen.playford at stfc.ac.uk](mailto:helen.playford@stfc.ac.uk)

Thu Jun 11 11:05:59 BST 2015

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Hi Ali,

Thanks very much for providing those instructions, which explain the format of the RMCPProfile Bragg input files.

I would like to note that if using neutron data the program data2config can be used instead of get_gsas_bragg to produce the necessary files (there are instructions in the manual). This program sometimes has bugs of its own, but is definitely worth a try.

Since Ali is primarily a neutron user, I would also add that (understandably) his instructions don't cover the format of the .xray file which is required if you are using RMCPProfile with X-ray data. The format of this file is incredibly specific and I do not recommend trying to create it manually. If bugs in get_gsas_bragg cause issues with X-ray data I would urge the person to get in touch with us via the mailing list.

Best wishes,
Helen

From: rmcprofile-users [mailto:[rmcprofile-users-bounces at rmcprofile.org](mailto:rmcprofile-users-bounces@rmcprofile.org)] On Behalf Of Ali Shehu
Sent: 11 June 2015 10:12
To: [rmcprofile-users at rmcprofile.org](mailto:rmcprofile-users@rmcprofile.org)
Subject: Re: [RMCPProfile-users] R: Re: R: Re: get_gsas_bragg

Dear all,

As an alternative to the get_gsas_bragg.exe program, constructing the gsas bragg files manually, following a few simple instructions (attached), proved rather easy to do and more beneficial in terms of understanding.

Regards

Ali Shehu
2nd Year PhD Student
Group of Dr Isaac Abrahams & Prof Martin Dove

SBCS and The School of Physics & Astronomy
Queen Mary University of London
Mile End Road, London, E1 4NS

From: rmcprofile-users <[rmcprofile-users-bounces at rmcprofile.org](mailto:rmcprofile-users-bounces@rmcprofile.org)> on behalf of [helen.playford at stfc.ac.uk](mailto:helen.playford@stfc.ac.uk) <[helen.playford at stfc.ac.uk](mailto:helen.playford@stfc.ac.uk)>
Sent: 11 June 2015 09:45
To: [rmcprofile-users at rmcprofile.org](mailto:rmcprofile-users@rmcprofile.org)
Subject: Re: [RMCPProfile-users] R: Re: R: Re: get_gsas_bragg

Dear all,

It seems like this is more common than I had realised - several people have emailed me as a result of this discussion to say they are also having this problem.

On Windows it seems that the version of GSAS/EXPGUI used may be causing problems. On my machine I am running revision 1225, which seems to work, and indeed the tutorial files would have originated from my version. Another user reports that revision 1188 does not work, so this is definitely something to check. You can go to Help > About in EXPGUI to find which revision you are using. (It's possible that this is an issue on Mac too, with revision 1175 reported to work and revision 1251 reported not to work).

Other things that can cause problems is if the program finds unexpected characters in the file, such as if your element symbols are of the type "O-2", and I've heard some reports that choosing too small a value for minimum d-spacing can cause crashes. I'm sorry that I can't give more specific advice.

If anyone has specific examples of non-working files I'd be very happy to field them and see if they run successfully on my setup. To avoid clogging up the list pages it might be best if you send them directly to me, or to [rmcprofile-users-owner at rmcprofile.org](mailto:rmcprofile-users-owner@rmcprofile.org)<mailto:[rmcprofile-users-owner at rmcprofile.org](mailto:rmcprofile-users-owner@rmcprofile.org)>.

Best wishes,

Helen

From: rmcprofile-users [mailto:[rmcprofile-users-bounces at rmcprofile.org](mailto:rmcprofile-users-bounces@rmcprofile.org)] On Behalf Of Giorgia Confalonieri
Sent: 09 June 2015 10:55
To: [rmcprofile-users at rmcprofile.org](mailto:rmcprofile-users@rmcprofile.org)
Subject: [RMCProfile-users] R: Re: R: Re: get_gsas_bragg

I think that this could be the problem, but I don't know how to solve it (I'm running on windows7).

Exactly as in the tutorial, Gsas is in a C folder so it should be rather simple to "find" it.

Now I have copied get_gsas_bragg.exe in the example folder, it has seemed to work but at the end it returned me the same error (attached).

Thank you

Giorgia

Il 09/06/15 10:49, [helen.playford at stfc.ac.uk](mailto:helen.playford@stfc.ac.uk)<mailto:[helen.playford at stfc.ac.uk](mailto:helen.playford@stfc.ac.uk)> ha scritto:

Dear Giorgia,

That's strange. The files from example 6 work fine on my computer, so I'm not sure what could be

wrong!

Is it possible that the get_gsas_bragg.exe is not finding the GSAS program itself? What OS are you running on?

Best wishes,

Helen

From: rmcprofile-users [mailto:rmcprofile-users-bounces_at_rmcprofile.org] On Behalf Of Giorgia Confalonieri
Sent: 09 June 2015 09:07
To: rmcprofile-users_at_rmcprofile.org<mailto:rmcprofile-users_at_rmcprofile.org>
Subject: [RMCPProfile-users] R: Re: get_gsas_bragg

Dear Helen

Thank you for your answer.

I have the same problem with the example 6. Every time that I try to execute get_gsas_bragg, it creates get_bragg_tempy.hst and get_bragg_tempy.temp and then stops with the error:

```
forrt1: severe(24): end-ofofile during read, unit 11, file get_bragg_tempy.hst
```

In any case I have attached the files to this mail.

Best regards

Giorgia

Il 09/06/15 09:49, helen.playford_at_stfc.ac.uk<mailto:helen.playford_at_stfc.ac.uk> ha scritto:

Hi Giorgia,

Looks like something is going wrong when the program tries to read your GSAS file. Could you please send me your files so I can try to see what's going wrong?

Best wishes,

Helen

From: rmcprofile-users [mailto:rmcprofile-users-bounces_at_rmcprofile.org] On Behalf Of Giorgia Confalonieri
Sent: 08 June 2015 13:05
To: rmcprofile-users_at_rmcprofile.org<mailto:rmcprofile-users_at_rmcprofile.org>
Subject: [RMCPProfile-users] get_gsas_bragg

Dear all

I'm trying to perform my first rmc refinement, so obviously I'm not an expert.

I have a big problem using get_gsas_bragg.exe (I have xray data) to extract .bragg,.back etc.

The error message is:

```
forrt1: severe(24): end-ofofile during read, unit 11, file get_bragg_tempy.hst
```

Could you help me?

Thank you

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Giorgia Confalonieri

PhD Student

Dept.: Scienze della Terra

Università degli Studi di Milano

email: giorgia.confalonieri@unimi.it<mailto:giorgia.confalonieri@unimi.it>

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email: giorgia.confalonieri@unimi.it<http://www.unimi.it/13084.htm?utm_source=firmaMail&utm_medium=email&utm_content=linkFirmaEmail&utm_campaign=5xmille>

rmcprofile-users mailing list

rmcprofile-users@rmcprofile.org<mailto:rmcprofile-users@rmcprofile.org>

<http://lists.rmcpfile.org/mailman/listinfo/rmcpfile-users>

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