



# Agenda

---

<b>Meeting title:</b>	CCP4 Working Group 2 meeting	
<b>Date:</b>	Wednesday 8th June 2016	<b>Time:</b> 11:00 – 16.00
<b>Location:</b>	Birkbeck, University of London, Geology room 612 (entry from Torrington Square)	
<b>Circulation:</b>	ccp4wg2@stfc.ac.uk	
<b>Present:</b>	Charles Ballard (CB), Arnaud Basle (AB), Dave Brown (DB), Paul Emsley, Phil Evans, Mike Hough, Ronan Keegan, Eugene Krissinel, Ed Lowe, Marc Morgan, Stuart McNicholas (SMN), Andrew Purkiss (AP), Kushwant Sidhu, Kyle Stevenson, Ivo Tews (ITE), Ville Uski, David Waterman (DW), Keith Wilson (KSW), Pamela Williams	

---

Please arrive for coffee at 10:30.

Directions <http://www.bbk.ac.uk/geology/contact-us/how-to-find-us>

WG2 agenda (only WG2 members)

1. Approval of minutes from the London WG2 meeting 2/3/16
2. Chairs report (Ivo Tews)
3. Acta Cryst Proceedings Issue “Protein-Ligand Complexes” (Paul Emsley)
4. Conferences and workshops (Charles Ballard)
5. Web pages (Charles Ballard)
6. Planning of the CCP4 SW2016 “From Crystals to Structure” (Keith Wilson, Mike Hough)
  - a. Proposed session structure
  - b. Proposed speakers
  - c. Plans for the Acta Cryst Proceedings Issue

Lunch

CCP4 v.7 and Gui2 – experiences, uptake, comments, feedback

7. What’s New in CCP4 Core Group, CCP4 7.0 (Eugene Krissinel)
  8. Xia2-DIALS interface in i2 (David Waterman)
  9. Gui2 comments and feedback from users (Ivo Tews)
  10. Practical example of GUI2 used for students (Ed Lowe)
  11. ccp4i2 updates (Stuart McNicholas)
  12. AOB
13. Take note of the date of the next meeting (proposal 21.9.2016)

# Minutes

## 1. Approval of minutes from the London WG2 meeting 2/3/16

The minutes from the London WG2 meeting 2/3/16 were approved.

## 2. Chairs report (Ivo Tews)

WG2 welcomes new members who have signed up; both receiving the mailing list and in attendance. WG2 focuses on “practicing crystallographers” in its constituency; while giving programmers the opportunity to discuss new developments, WG2 thus offers the option to discuss with users / the community.

The experience in the past period has been that feedback to introduction of CCP4v7 and Gui2 has been very limited through the CCP4bb channel – this prompts WG2 to take advantage of the targeted audience.

IT proposed a new form of communication. In an effort to reach “practicing crystallographers” across the UK who are not necessarily part of WG2, PI and/or alternative contacts from Diamond bags have been contacted; this has required consideration of the data protection act, and is done in a way to avoid soliciting / spamming; these contacts are consensual, not disclosed to anyone, and returns anonymised. Rather than doubling up from WG2 and disseminating the same information, this channel was (and is to be) used only to advertise offers that are outside of WG2, e.g. as the Gui2 feedback session (during this meeting) and the bring-your-own-data DIALS workshop (next WG2 meeting), and limited to very few mails per year (max. 4). The advantage is user feedback and engagement without requiring WG2 membership.

This proposal was discussed.

DB: number and regional distribution of BAG?

ITE: tried to contact all Diamond BAGs, but UK uses only.

KSW: Is anonymous bad? Feedback without being able to communicate back is not helpful, and inf act other channels to give feedback exist (CCP4 e mails)

AB: the WG2 list is limited to about 60 people. Who else?

ITE: a list of BAGs has been created, with about dozen responders and eight non-responders.

IT: proposal to use a similar structure in future with a WG2 (closed) meeting in the morning, with an open WG2 afternoon session to discuss developments with users – keep this structure?

DB: it is a good idea to get better engagement with new people and interactions with developers.

SMN: yes good idea. We should go north and west as well.

DB: Consider that a roadshow could be done.

CB: Moving around works well with the students.

AP: should developers going to the beamline?

DB: beamline scientist is the support.

DW: we cannot get to the beamline.

WG2 was represented by the chair at the Developers meetings Mar 13-15<sup>th</sup> 2016 and the Exec meeting Mar 15<sup>th</sup> at Coseners. Planned is presentation at the SWSBC at Portsmouth, 27-28.6.2016.

### 3. Acta Cryst Proceedings Issue “Protein-Ligand Complexes” (Paul Emsley)

While several papers are accepted, some authors are still pending submission, and these will be contacted. The total at this stage is six papers out of twenty (1 declined and 1 elsewhere). The Acta Cryst special issue usually has 17-18 papers.

### 4. Conferences and workshops (Charles Ballard)

CB reported on planning of meetings (ACA 22-26.7.16, BSR 21-24.8.16, ECM 28.8-1.9.16, CCP4SW 8-10.1.17, ACA 2017. IUCr 2017); CCP4 has a stand at ACA and IUCr but this option is not viable for other meeting due to cost (ECM).

KSW: What about European users?

DW: CCP4 is present through the Diamond Workshops, European users are coming.

CB: CCP4 sponsors 3 meetings (rapiddata Stanford, SWSBC and Carlisle).

KSW: CCP4MG workshop at Carlisle.

AB/SMN: should be feasible.

ITE: during meetings, workshops on software are receiving good comments from users; plan for this at the SWSBC. This is generally better value for money than a stand.

CB reported on planning of workshops (CCP4 India 15-19.2.16 – 50 students; IFSC/CCP4 Brazil 4-14.4.16 – 20 students; CCP4-APS 21-29.6.16 – 20 students; BCA/CCP4 summer school DLS 21.-26.8.16 – 20 students; DLS-CCP4 Dec 2016 – 20 students; CCP4-Spring8 23-27.1.2017 – 20 students).

### 5. Web pages (Charles Ballard)

STFC is supporting the webserver on their hardware. CCP4 will be responsible for content and the virtual machine management. The website managed would be through Drupal ([www.drupal.com](http://www.drupal.com)). The system is built around modules and templates, and use is similar to WordPress.

Progress is slow due to lack of resources. Initial main page building failed due to javascript. Javascript is required for stuff behind the scene. Timeline?

### 6. Planning of the CCP4 SW2016 “From Crystals to Structure” (Keith Wilson, Mike Hough)

The SW2017 will focus on ccp4 programs. Keith and Mike presented the proposed programme and potential speakers were discussed (not minuted):

- Measuring intensities
  - Synchrotrons
  - Dials and XIA2
- Intensities
  - Aimless
  - Multi crystal
  - Experimental phasing
- Experimental phasing pipelines
  - Crank2

- Phase EP
- Model building
- Coot
- Molecular Replacement
  - Phaser
  - MrBump
  - Restrains refinement
  - Local model help
- An initio
  - Ample
  - Acrimboldo
  - From fragments
- Session 6
  - Ligands
  - Validation
  - Deposition
  - Cloud

DB: topics and flow look good.

ITE: Points to discuss: Are we lacking anything? How main-stream is *ab-initio*? What makes good papers?

## 7. What's New in CCP4 Core Group, CCP4 7.0 (Eugene Krissinel)

Updates of CCP4 installations. About 80% of CCP4 installations are not updated. One reason why we would not detect updates is that user might install CCP4, and at a later stage download a newer version and re-install when needed.

New is a collaboration of CCP4 with Global Phasing to develop updated libraries to be used by both parties. Marcin Wojdyr will be starting in July 2016 on this.

Ville Uski is involved with services in the Cloud. Currently there are three different approaches: CCP4 online, remote desktop (access to Diamond MX beamlines STFC computing resources), and remote job submission.

<https://daas.scd.stfc.ac.uk> (needs diamond FedID) can be tested and have webdav but need vpn to connect to. A remote task is being developed in i2 (Liz). Restful api for job submission in progress.

## 8. Xia2-DIALS interface in i2 (David Waterman)

Technical implementation: Xia2 and cctbx use .phil files so it was necessary to make i2 understand .phil (generic) def.xml.

We should now be able to auto-generate the interface; problems remaining are nested containers (from .phil). Wrap around the interface is xia2\_dials – limitation: only one widget per line (too many for the advanced tab). Some issues such as untrusted rectangle, i.e. Xia2 dependence on unit cell and space group.

The reports rely on the aimless pipeline (not the xia2 task)

## 9. Gui2 comments and feedback from users (Ivo Tews)

Feedback has been directed to the Gui2 team.

## 10. Practical example of GUI2 used for students (Ed Lowe)

Ed is running a crystallography course for students and just updated the practical to gui2. 26 students attended, many of them inexperienced in crystallography.

The practical covered data processing and sad phasing:

- Inspect data with imosflm, autoindexing with xia2 dials
- HA site determination with shelx, Phaser EP, ncs with parrot
- inspect map in coot, autobuild in buccaneer (students liked the generated pictures).
- Molecular replacement followed Arlie's tutorial

The student feedback was very positive. It was helpful to be consistent throughout. GUI2 ran well on vm linux machines on windows with 8 GB of memory.

## 11. ccp4i2 updates (Stuart McNicholas)

GUI2 needs to be configured for mechanism and machines. The user will pick the cluster and provide user name and password. Liz and Ville tested this on Harwell machines, and it should work for most installations.

Importing ccp4i project help should be improved for guidance.

Jon Aguirre's new privateer can choose expression system to draw glycan in 2D.

Stuart McNicholas' new CCP4MG glycoblocks are a new representation including stacking.

CCP4MG MrBump task (can use slider to fine tune result from Gesamt) waiting to be rolled for next cpp4 update or further development.

## 12. AOB

None.

## 13. Take note of the date of the next meeting.

Possible dates are June (suggested dates: 21.9.2016), Locations suggested: London or DLS.

Google poll to agree on date and location to follow.