Arbeitsgemeinschaft
für Kristallographie
und Strukturchemie

RWTH AACHEN UNIVERSITY

Prof. Dr. Ulli Englert
Institut für Anorganische Chemie
Landoltweg 1
52056 Aachen

Telefon: +49 241 80-94666
Fax: +49 241 80-92288
ullrich.englert@ac.rwth-aachen.de

To our clients and cooperation partners

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Dear clients and cooperation partners,

the following short text is intended to help you with the results from diffraction experiments.

We distinguish two modes of interaction with our fellow scientists: a) data collection/integration or b) data collection/integration/structure solution/refinement/interpretation/assistance for publication; both cases are explained below.

a) As a general rule, we do NOT expect to be co-authors of your papers if we "only" perform data collections for you and "only" do integration/data reduction/scaling. Rather, you and your group leader will decide about and be responsible for (non-)publication of the results.

Diffractometers are expensive, both in terms of acquisition and maintenance. Nevertheless, we do not charge money for data collection - most expenses are in general covered by the Institute of Inorganic Chemistry. You or your group leader will not receive a bill without prior notice. We may, however, charge a contribution to diffractometer maintenance and consumables such as liquid nitrogen from those groups outside IAC who regularly receive diffraction data. The group leaders will be informed about any such contribution well before billing.

We do not deliberately delete diffraction data, but we decline responsibility for long term data storage. In 2013, we were asked to urgently re-provide data collected in 1991; unfortunately, the magnetic tape recorded in these days resulted illegible. Shelf life for CDs etc. will be shorter. Please store your results in a safe place and find your own answer to the question whether the hard disk of your computer is suitable and will be regularly backed up. All B.Sc., M.Sc., Ph.D. candidates and post docs should forward a copy of their results to their group leader.

Each structure is assigned a data collection code (e.g. **w15_40**) consisting of

- an initial letter: it stands for the operator (**w**illiam in the example above)
- a two digit number which denotes the year in which the data were collected (20**15** in the example above)
- an underscore **_**
- a number which uniquely identifies the data set (**40** in the example above).

Please cite this code if you need additional information or if a data collection should be repeated. You will receive the results of your diffraction experiment by email or as a gigamove download link; please note that such download links expire after a week or two.

What do you get?

In general, the following files will be transmitted; <code> stands for the data collection code explained above, e.g. w15_40:

- intensity data after scaling/absorption correction, file name <code>.hkl

- unit cell data matching the setting of the intensity data above, <code>.ins

- raw intensity data containing direction cosini, <code>m.raw; these data have not been scaled/absorption corrected and allow you to test your own absorption correction/scaling strategies and programs

- crystal information file <code>.pcf with crystal dimensions, colour, shape, data collection temperature, number of reflections and theta range used to subtend the unit cell

- scaling/absorption correction logging, <code>.abs

- scaling/absorption correction graphics, <code>.eps

- final orientation matrix, <code>m.p4p

The files above will allow you to solve, refine, interpret, deposit and publish your crystal structure. Please look at your files and let us know if anything is missing - speak to us or your group leader if you are in doubt. Do not postpone a discussion about your results to the time you want to write up your thesis or your boss wants to publish! We do not feel obliged to search through thousands of intensity data collections and perform urgent calculations based on a phone call of the type: "Eh, you remember that one ferrocene derivative... one of you guys, I do not remember who, did the structure, probably four or six years ago. I would like to publish that now, in fact the paper is finished, I urgently need the interplanar angle between the Cp ligand and the benzene ring..."

b) In contrast to the situation above and in agreement with general practice, those of us expect to be co-authors in your publications who make RELEVANT contributions to a manuscript such as structure solution, refinement and interpretation. Like most scientists contributing to publications, we insist in looking at all manuscripts carrying our name.

In addition to the files explained above, you will receive feedback whether or under which conditions your results match the requirements for publication. In most cases you will receive a file <code>.cif ready to be submitted for publication and/or deposition with the CCDC. In case b) we will help you to deposit your data, draft the experimental part of your publication and assist with interpretation and graphical representation of your structure for the manuscript and/or the supporting information.

As often in life, there may be borderline situations in-between the cases a) and b); they will be settled by mutual agreement.