The Presentation of Results

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The final stage of a crystal structure analysis is its presentation, which could occur within your own research group, as a conference poster or oral contribution, or as a refereed article in a journal. In each case the requirements are different and you must tailor the presentation to the medium used. As with all communication skills the presentation of crystallographic results improves with practice. In this context, presentation covers almost everything that happens to a structure after the refinement is satisfactorily converged and the structure validated.

Key points

Journal guidance. The reporting of structural results in crystallographic or chemical journals is usually guided by the relevant *Notes/Instructions/Guidance for Authors* provided by these journals. It is an obvious point, but sometimes overlooked, that you should consult such guidance before you begin writing and assembling the article.

Selection of material. There has been a marked trend away from publishing primary data such as coordinates and displacement parameters. With strict page limits in force on some journals, even more careful selection of material for inclusion in the main text and in the supplementary information is vital, as is the choice of effective graphical abstracts.

Graphics programs. There is a wide variety of programs which can produce high-quality illustrations of crystal structures. Many of these are free, at least for academic users. Some are standalone while others are part of comprehensive packages. Display styles include ball-all-stick, displacement ellipsoid, polyhedral and space-filling. Compatibility is an important consideration: can the program you want to use read the relevant input format and output the graphics in the format required? Molecular representations may be less appropriate for inorganic compounds than polyhedral plots in which neighbouring polyhedra are linked through their vertices, edges or faces to build up the structure. Links to relevant programs will be provided.

View direction. The viewing direction is an important consideration: it might be along a unit cell axis or other crystallographic direction, or with respect to molecular features. It may help to start looking along the direction perpendicular to the mean plane through all the non-H atoms, then make small rotational adjustments to optimise the view.

Connectivity information. For the majority of drawings, composed from atoms and the bonds linking them, the program depends on a connectivity array calculated using values for covalent or other radii appropriate to each atom. The default array may work well for organic compounds but manual intervention is more likely to be needed for organometallic and inorganic compounds.

Packing diagrams. Packing diagrams pose particular challenges because the default contents and view direction are seldom satisfactory. How can such diagrams be designed in order to bring out the points you wish to illustrate without introducing unnecessary clutter? Packing diagrams and their captions are frequently of poor quality and low information content.

Three dimensions. Representing a three-dimensional structure in two dimensions involves loss of information and the results can be quite misleading. Techniques which aim to recover some of this information include depth cueing, the use of perspective, bond tapering, hidden line removal, the use of shading or highlights and the induction of stereopsis.

Colour. When used appropriately, colour can greatly enhance the attractiveness and impact of illustrations. Note that there are loose conventions for atom colours: their use can convey additional information but conversely flouting these conventions may confuse your readers.

Labelling. Unless colour or shading has been specifically used to identify atom types, suitably-sized and carefully-placed labels are essential. Sometime only a subset of atoms need be labelled (*e.g.*, heteroatoms in an organic structure, metal and donor atoms in a coordination complex), but any atoms referred to in the text or in a table should be identified. Other textual information usually appears in the figure caption.

Hints. A set of hints for producing effective illustrations will be provided in the lecture.

Tables of results

The tables produced at the end of the structure refinement will usually comprise:

- a summary of crystal data
- fractional atomic coordinates (with s.u.s) and U_{eq} values for the non-H atoms:
- atomic displacement parameters – normally U^{ij} – with s.u.s;
- fractional atomic coordinates and U_{iso} values for H atoms
- molecular geometry parameters (bond lengths, valence angles, torsion angles)
- intermolecular contacts, least squares mean plane data, *etc*.
- structure factor tables.

The content of tables. Tables of molecular geometry parameters will comprise your selection of parameters based on the chemical nature of the compound and the structural features which you want to emphasise. Parameters which have been constrained during refinement, or which are unreliable because they fall in a region affected by disorder, are routinely omitted. Only one representative of a group of symmetry-equivalent parameters needs to be included, but you should ensure that significant parameters arising from the application of symmetry, or which lie outside the conventional limits, are included.

Hints on presentation. Specific advice will be presented regarding presentation in different contexts, including in scientific journals, in theses and reports, on posters, as oral presentation and on posters.

Archiving of results. Hopefully the results of your structure determinations will soon be published and partially archived in a database, but you must keep your own copies of all relevant files and other information safely and in an accessible form. Funders or regulatory authorities may demand access to these data long after publication. When archiving data the main considerations are those of security and accessibility: you must have a suitable, robust strategy in place as a precaution against risks such as hard drive failure, computer viruses, fire and flood.