General Problems

The use of several programs on several platforms (PC/MAC) often ends in incompatibility problems with different graphic formats. Keeping the high quality of a graphic through the various steps, which are needed to create a publication-ready picture, is often nearly impossible.

=> Work only with common graphic file formats available on all platforms that keep the quality !

a) **HPGL** (**H**ewlett **P**ackard **G**raphic **L**anguage); common extensions: .hgl or .hpg
b) **EPS** (**E**ncapsulated **P**ostscript); common extension: .eps

General recommendations

a) Don't use *Cache* for creating ORTEP plots on paper! The pictures look very nice on the screen, but *Cache* is unfortunately not able to export the pictures in reasonable and easy to handle high quality graphic formats.

b) Don't use "*Copy and Paste*" for pictures! High quality informations often get lost during this procedures and the result is a "screen shot" like resolution.

c) Don't use *Chemdraw* for importing ORTEP plots as long as the PC version is not able to handle *eps*-files in a reasonable way (incompatibility problem MAC/PC!)

General procedure

Step 1: Generating the ORTEP plot - use *ORTEP III* **for Windows**

The ORTEP (<u>O</u>ak <u>R</u>idge <u>T</u>hermal <u>E</u>llipsoid <u>P</u>lot) program is a computer program for drawing crystal structure illustrations. Ball-and-stick type illustrations of a quality suitable for publication

are produced <u>with either spheres or thermal-motion probability ellipsoids, derived from anisotropic temperature factor parameters</u>, on the atomic sites.

ORTEP is definitely not the highest sophisticated and most user friendly program, but is able to write nice high quality *hgl*-files and *eps*-files and is able to handle X-ray data (symmetry operations etc.) properly.

Please open a <u>copy</u> of your *res*-file (stored in the X-ray-archive on the *Cache*-PC) with *ORTEP III*. Use the default settings of the program (ellipsoid probability = 50%; plot line width = 1; style = <u>organic</u> or inorganic). When the orientation of the molecule is set, please write a *hgl*-file or an *eps*-file. It is better not to use the routines of *ORTEP* to generate the labels of atoms.

Step 2: Manipulating and labeling the plots with **Adobe Illustrator** (Mac or PC)

Adobe Illustrator is one of the best programs for handling and manipulating eps-files. If you have an eps-file created by *ORTEP*, you can directly open it. <u>A small disadvantage here is, that *eps*-pictures from *ORTEP* might have very thick drawing lines, but these can be reduced to a nicer scale by *Illustrator*</u>.
If you want to avoid this, create a *hgl*-file with *ORTEP III*. This file can be converted easily to an *eps*-file with *CorelDraw* on a PC or *LaserPlot* on a Mac.

After labeling the structures with the *Illustrator* text routines please save the files in the <u>"Illustrator EPS"</u>-format. This format can be easily imported into *MS Word* for adding the captions etc.

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Remarks

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1. Do all graphic manipulations and changes within *Illustrator* and <u>keep this *eps*-files</u>! If you don't have to add captions etc. in JAG's preferred layout style, you are finished here. You can print these files directly always in best quality on any postscript printer on all platforms.

2. If you have to add text - use only *MS Word* and import the *eps*-graphics.